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Additional Information

Computational study on the influence of nozzle eccentricity in spray formation by means of Eulerian Σ - Y coupled simulations in diesel injection nozzles

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Abstract

The present work analyses the effect of the eccentricity of diesel nozzle orifices over the spray behaviour by means of CFD simulations. Several orifice geometries with varying horizontal eccentricity (from 0.50 to 0.94) are selected. Their performance is assessed at a high injection pressure of 200 MPa, a 3 MPa back-pressure and non-evaporative conditions. The nozzle flow characteristics, including cavitation modelled by a Homogeneous Relaxation Model (HRM), are accounted for in the spray performance by means of a Σ - Y model. The code is validated via two reference nozzles, the so called "Spray A" of the Engine Combustion Network plus a second nozzle from a production injector, and then extended to the eccentric geometries. The results and discussions include spray angle and penetration, air entrainment and flow parameters of the nozzle inner conditions versus the eccentricity value.

Keywords: Sigma - Y model, HRM, eccentricity, diesel, spray, atomization

1. Introduction

As the standards applied to combustion engines emissions become more stringent, the need to produce cleaner combustion systems compatible with future climatic requirements is critical. Diesel engines have been widely used thanks to their potential to reduce CO_2 emissions, one of the most significant contributors to global warming effect. However, concerns about their capability to meet future NO_x and particulate matter emissions regulations have arisen over the last years. Even if these pollutants can be substantially reduced by means of aftertreatment systems (such as Diesel Particulate Filters -DPF-, Lean- NO_x Trap-LNT- or Selective Catalytic Reactors -SCR-), the origin of the emissions must be also controlled in order not only to reduce them, but also to keep under control the cost, size, durability and fuel consumption impact of the

19 aforementioned elements. While Exhaust Gas Re-
20 circulation (EGR) can be used to mitigate NO_x
21 emissions thanks to the lower combustion tempera-
22 ture, its usage is limited due to the subsequent in-
23 crease of the particulate matter (mainly composed
24 of soot). However, soot formation is controlled by
25 the air-fuel mixing process, which is mainly a result
26 of the injection pressure and the morphology of the
27 injector and chamber geometry (Arai, 2012; Hey-
28 wood, 1988; Lefebvre, A., McDonell, 2017). Addi-
29 tionally, the fuel-air mixing controls the combus-
30 tion timing and duration, affecting the indicated
31 efficiency, as well as the flame distance to the cylin-
32 der walls, impacting heat transfer losses.

33 Since the 1970's the study of the parameters that
34 characterize the spray performance has been a con-
35 stant research topic with the aim of increasing ef-
36 ficiency while reducing emissions. First works by
37 Wakuri et al. (1960), the extensive studies by Hiroy-
38 asu et al. (Hiroyasu, 2000; Hiroyasu and Arai, 1990;
39 Hiroyasu and Kadota, 1974; Hiroyasu and Miao,
40 2003) and several others like Reitz et al. (Reitz,
41 1987; Reitz and Bracco, 1982; Reitz and Diwakar,
42 1987) postulated the importance of the spray me-
43 chanics, specially the relationship between the tip

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Nomenclature

| | | | |
|-------------|---|------------------|---|
| A | Area | $RANS$ | Reynolds Averaged Navier-Stokes equations |
| a | Ellipse semi-major axis | RNG | Re-normalization Group |
| AMR | Adaptive Mesh Refinement | S_i | Source term |
| b | Ellipse semi-minor axis | Sc | Schmidt number |
| c | Focal length | T | Temperature |
| C_a | Area coefficient | \tilde{u}_i | Velocity component |
| C_d | Discharge coefficient | u_{eff} | Effective velocity |
| C_v | Velocity coefficient | u_{th} | Theoretical velocity |
| C_Σ | Model coefficient for Σ | V | Volume |
| D | Mass diffusion coefficient | XY_{plane} | Perpendicular to the ellipse major axis |
| D_o | Nozzle outlet diameter | \bar{Y} | Liquid volume fraction |
| D_Σ | Diffusion coefficient for Σ | \tilde{Y} | Liquid volume fraction, Favre averaged |
| D_{eq} | Equivalent diameter, defined as $D_{eq} = D_o \sqrt{\frac{\rho_l}{\rho_a}}$ | Y | Mass fraction |
| e | Eccentricity | ZY_{plane} | Perpendicular to the ellipse minor axis |
| e | Specific energy | α | Void fraction |
| F | Cavitation parameter of the HRM model | α_1 | Calibration parameter |
| h | Enthalpy | α_2 | Calibration parameter |
| HRM | Homogeneous Relaxation Model | δ_{ij} | Kronecker delta |
| \bar{k} | Turbulent kinetic energy | $\bar{\epsilon}$ | Turbulent energy dissipation |
| K | Temperature diffusion coefficient | φ | Non-dimensional pressure ratio |
| \dot{M}_f | Momentum flux | μ | Viscosity |
| \dot{m}_f | Mass flow | μ_t | Turbulent viscosity |
| M | Momentum | ν_T | Kinematic turbulent viscosity |
| m | Mass | ρ | Global density |
| P | Pressure | Σ | Surface are density |
| PMD | Projected mass density | σ_{ij} | Viscous stress tensor |
| R | Radio | θ | Time scale factor |
| r_{eq} | Equivalent droplet radio | | |

44 penetration, the spray angle and the air entrainment. 45 Different optical diagnostics have been developed 46 to evaluate the primary atomization and initial 47 spray formation process (Desantes et al., 2011; 48 Dumouchel, 2008; Manin et al., 2014), the fuel-air 49 mixing (Espey et al., 1997; Schulz and Sick, 2005) 50 and the combustion development (Desantes et al., 51 2018; Idicheria and Pickett, 2011). The evolution 52 of computational fluid dynamics in the recent years 53 has made possible to study in further details the 54 importance of the nozzle geometry in the atom- 55 ization process (Anez et al., 2018; Desjardins and 56 Pitsch, 2010; Salvador et al., 2014, 2015b). In this 57 sense, approaches such as the $\Sigma - Y$ model (Val-

58 let and Borghi, 1999; Vallet et al., 2001) which 110
59 allows a coupled flux between nozzle and spray 111
60 through a Eulerian-Eulerian simulation (Desantes 112
61 et al., 2016a; Wang et al., 2011; Xue et al., 2015). In 113
62 this model, flux phases are considered as a pseudo- 114
63 fluid inside a single velocity field. This method in- 115
64 troduces the possibility of simulate cavitation phe- 116
65 nomena if the geometry is prone to cavitate. In this 117
66 sense, several authors such as Zhao et al. (2014) and 118
67 Battistoni et al. (2015) used an Homogeneous Re- 119
68 laxation Model to evaluate cavitation phenomena 120
69 in nozzles. 121

70 Already decades ago, works by Sforza et al. 122
71 (1966) and Trentacoste and Sforza (1967) made 123
72 first approximations to the aspects of jets produced 124
73 by elliptical nozzles. Hussain et al. (Husain and 125
74 Hussain, 1991; Hussain and Husain, 1989) and Ho 126
75 and Gutmark (1987) analysed also these jets from 127
76 a theoretical perspective. More recently, studies 128
77 about elliptical nozzles applied to spray mechan- 129
78 ics revealed that this particular shape was able 130
79 to improve the general dispersion of the injected 131
80 fluid (Yunyi et al., 1998). Lee et al. (2006) per- 132
81 formed comparisons between elliptical and cylin- 133
82 drical single-hole nozzles and found an improved 134
83 spreading angle, specially in the plane correspond- 135
84 ing to the minimum diameter. Similar results were 136
85 reported by Yu et al. (2018), showing a lower pene- 137
86 tration in favour of a wider angle and then a greater 138
87 atomization effect associated to elliptical single-hole 139
88 nozzles. Hong et al. (2010) studied cavitation phe- 140
89 nomena inside transparent elliptical nozzles, con- 141
90 cluding that longer cavitation fields (up to the ori- 142
91 fice outlet) were appearing. Based on the work by 143
92 Hong et al., Ku et al. (2011) applied CFD tech- 144
93 niques in order to verify the relationship between 145
94 the internal flow and the behaviour of the spray. 146
95 Their investigation showed how cavitation takes 147
96 place in the major axis limits due to a greater con- 148
97 traction of the stream-lines in that zone for single- 149
98 hole nozzles. The internal profiles of the CFD sim- 150
99 ulations related the turbulence subjected to cavi- 151
100 tation to a greater spreading angle in the major 152
101 axis plane. Finally, some approximations to real 153
102 diesel engines were made by Matsson and Ander- 154
103 sson (2002), accounting the impact on emissions 155
104 of elliptical geometries, with a general decrease of 156
105 NO_x emissions and fuel consumption for elliptical 157
106 geometries, but with varying smoke production de- 158
107 pending on the aspect ratio value. 159

108 Despite the previous works describe some of the 160
109 physics related to the impact of elliptical orifices on 161

nozzle flow and spray formation, most of them may 110
not be fully representative from a practical point 111
of view. On the one hand, most of the studies 112
are performed for single-hole axi-symmetric nozzles. 113
However, diesel engines require multi-orifice noz- 114
zles, which are affected by the change of direction 115
of the flow induced by the inclination of the orifices' 116
axis compared to the injector. On the other hand, 117
nozzle sizes within literature are usually larger than 118
a representative diesel nozzle ($< 0.2mm$). A first 119
approach to this more complex problem was de- 120
scribed by Molina et al. (2014). In their work, sev- 121
eral detailed CFD simulations were carried out in 122
order to clarify how the internal flow of a common 123
rail diesel injector with elliptical orifices could affect 124
the atomization, and an extrapolation to the effects 125
in the spray characteristics was made based on a 126
theoretical reasoning. The present paper intends 127
to get a deeper view into the effects of elliptical 128
nozzles over the spray by means of advanced cou- 129
pled internal-external flow simulations. This will 130
also allow to understand some of the effects de- 131
scribed in the literature. On the basis of a cavi- 132
tating cylindrical nozzle whose hydraulic behaviour 133
is known, six elliptical geometries have been mod- 134
elled. The horizontal radius has been gradually 135
increased inducing eccentricity levels from 0.5 to 136
0.94, maintaining a constant outlet section, while 137
the rest of the geometrical morphology has been 138
kept as in the original nozzle. The validation of the 139
computational model has been carried out following 140
two lines of action. First, a non-cavitating single- 141
hole nozzle from the Engine Combustion Network 142
(<https://ecn.sandia.gov/ecn-data-search/>), named 143
Spray A, has been evaluated in terms of mass flow 144
rate, momentum flux, spray angle and projected 145
mass density. Then, a Homogeneous Relaxation 146
Model (HRM) used to predict cavitation perfor- 147
mance has been assessed against hydraulic exper- 148
imental data from a cylindrical multi-hole nozzle, 149
which is the same used as baseline for the rest of the 150
study. Once the models are validated, the perfor- 151
mance of the elliptical nozzles is analysed in terms 152
of the flow conditions at the nozzle outlet (mass 153
flow, momentum flux, liquid and vapour fractions, 154
radial and axial velocity profiles, etc), as well as 155
spray features (such as the spray angle, the air en- 156
trainment and the spray tip penetration). Several 157
discussions over the information available in liter- 158
ature have been exposed and the behaviour of the 159
simulations have been clarified. 160

The investigation has been divided into six sec-

162 tions. Section 2 introduces the computational 206
 163 model, while section 3 describes the employed 207
 164 methodology. It includes the description of the
 165 models, the geometries, fluid properties and the
 166 post-process and comparison techniques. Section 4
 167 discusses the validation of the model, including the
 168 description of the nozzle geometries used for this 208
 169 purpose (Spray A and a production multi-hole 209
 170 injector), the characteristics of the meshes and model
 171 constants configuration used. Section number 5
 172 shows the results for the six nozzles elliptical ge-
 173 ometries considered. All the nozzles have been com-
 174 pared relating their spray characteristics with the
 175 previous literature findings, paying special atten- 210
 176 tion to coherence between extracted properties at 211
 177 the nozzle outlet and the spray behaviour. The last
 178 section collects the main conclusions of the present
 179 work.

180 2. Model description

181 The coupling between the nozzle internal flow
 182 and the spray is made by means of a $\Sigma - Y$ atom- 212
 183 ization model. In this formulation, all the phases 213
 184 are treated as a pseudo-fluid with an unique veloc- 214
 185 ity field for vapour fuel, liquid fuel and chamber 215
 186 gas (Desantes et al., 2016a; Pandal Blanco, 2016). 216
 187 This approximation assumes that the exiting spray 217
 188 is characterised by large values of Reynolds and
 189 Webber numbers. From this point of view, big-
 190 ger scales of turbulence can be transported, while
 191 small unresolved scales are computed using stan-
 192 dard closure models. The dispersion of the liquid
 193 phase is then traced by means of a scalar function.
 194 This magnitude takes a value of 1 when only liq-
 195 uid exists, and 0 if there is only vapour phase. The
 196 transport equation for the liquid mass fraction on
 197 its Favre averaging form is:

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

198 where $\bar{\rho}$ denotes the density, \tilde{u} the axial veloc-
 199 ity, x the axial position and \tilde{Y} is the mean mass-
 200 averaged volume fraction defined as:
 201

$$\tilde{Y} = \frac{\overline{\rho_{liq} Y}}{\bar{\rho}}. \quad (2)$$

202 \bar{Y} being the volume fraction.

203 If an immiscible mixture is assumed for the two
 204 phases, the relation between the mass-averaged
 205

value of the liquid volume fraction can be related
 to the density by:

$$\frac{1}{\bar{\rho}} = \frac{\tilde{Y}}{\rho_l} + \frac{1 - \tilde{Y}}{\rho_g}. \quad (3)$$

An equation of state is then assigned to each
 phase:

$$\rho_g = \frac{P}{R_g T}, \quad (4)$$

$$\rho_l = f(p, T). \quad (5)$$

The energy transport equation only accounts the
 internal energy of the fluid, and stands as follows:

$$\begin{aligned} \frac{\partial \bar{\rho} e}{\partial t} + \frac{\partial \tilde{u}_j \bar{\rho} e}{\partial x_j} = & -P \frac{\partial \tilde{u}_j}{\partial x_j} + \sigma_{ij} \frac{\partial \tilde{u}_i}{\partial x_j} \\ & + \frac{\partial}{\partial x_j} \left(K \frac{\partial T}{\partial x_j} \right) + \frac{\partial}{\partial x_j} \left(\bar{\rho} D \sum_m h_m \frac{\partial \tilde{Y}_m}{\partial x_j} \right), \end{aligned} \quad (6)$$

Where Y_m and h_m are the mass fraction and en-
 thalpy for each species respectively, D is a mass dif-
 fusion coefficient, P is the pressure, σ_{ij} the stress
 tensor, e is the specific energy and T is the temper-
 ature. The relation between the different species is
 given by:

$$h(T) = \tilde{Y} \cdot h_l(T) + (1 - \tilde{Y}) \cdot h_g(T). \quad (7)$$

The turbulent term in the liquid mass transport is
 modelled as

$$\bar{\rho} \widetilde{u'_i Y'} = \frac{\mu_t}{Sc} \frac{\partial \tilde{Y}}{\partial x_i}. \quad (8)$$

Subsequently, the momentum conservation equa-
 tion can be written as:

$$\frac{\partial \bar{\rho} \tilde{u}_i}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i \tilde{u}_j}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial \sigma_{ij}}{\partial x_j} + S_i, \quad (9)$$

where σ_{ij} denotes the viscous stress tensor,
 equals to:

$$\sigma_{ij} = \mu \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) + \left(\frac{2}{3} \mu \frac{\partial \tilde{u}_k}{\partial x_k} \delta_{ij} \right), \quad (10)$$

μ is representing the viscosity and δ_{ij} is the Kro-
 necker delta.

Finally, the interphase surface area density is de-
 fined as the quantity of spatial surface per unit
 volume (Ishii and Hibiki, 2006; Vallet and Borghi,

1999). Hence, the transport equation associated to this scalar magnitude is:

$$\frac{\partial \tilde{\Sigma}}{\partial t} + \frac{\partial \tilde{u}_j}{\partial x_j} - \frac{\partial}{\partial x_j} \left(D_{\Sigma} \frac{\tilde{\Sigma}}{\partial x_j} \right) - C_{\Sigma} \tilde{\Sigma} \left(1 - \frac{\tilde{\Sigma}}{\Sigma_{eq}} \right) - S_{\Sigma_{evap}} - S_{\Sigma_{init}} = 0, \quad (11)$$

220 where

$$\overline{\Sigma_{eq}} = \frac{3\bar{\rho}Y}{\rho_l r_{eq}}, \quad (12)$$

$$S_{\Sigma_{evap}} = \frac{2\Sigma}{3\bar{Y}} S_{evap}, \quad (13)$$

$$C_{\Sigma} = \alpha_1 \frac{\tilde{\varepsilon}}{k'}, \quad (14)$$

$$r_{eq} = \alpha_2 \frac{\sigma^{3/5} (\bar{\rho}\tilde{Y})^{2/15}}{\tilde{\varepsilon}^{2/3} \rho_l^{11/15}}, \quad (15)$$

$$D_{\Sigma} = \frac{\nu_T}{Sc_{\Sigma}}. \quad (16)$$

221 D_{Σ} is a diffusion coefficient, Y is the volume frac-
 222 tion of fuel, $S_{\Sigma_{evap}}$ is a source term related to va-
 223 porization, $S_{\Sigma_{init}}$ is the initialization value, r_{eq} is
 224 the equilibrium radius for virtual droplets. Finally,
 225 α_1 and α_2 are model parameters subjected to cal-
 226 ibration. The terms above can be used to calcu-
 227 late equivalent droplet sizes as part of the transition
 228 chain to parcels in an hybrid Eulerian-Lagrangian
 229 model. Although this kind of comparison is beyond
 230 the limits of this paper, it is a good indication of
 231 the potential of the model.

$$S_{\Sigma_{init}} = \frac{\Sigma_{min} - \Sigma}{\Delta t} pos(\Sigma_{min} - \Sigma), \quad (17)$$

$$\Sigma_{min} = \sqrt{\alpha(1 - \alpha)} V^{1/3}, \quad (18)$$

$$pos(\Psi) = \begin{cases} 1 & \text{if } \Psi > 0 \\ 0 & \text{if } \Psi \leq 0. \end{cases} \quad (19)$$

232 In diesel engines, usual values for α_1 and α_2 are
 233 respectively 1 and 4 (Vallet et al., 2001; Wang et al.,
 234 2011). For a deeper mathematical explanation of
 235 the model and coefficients, previous work by Pandal
 236 Blanco (2016) can be consulted.

As stated during the introduction, the mass transfer between fuel vapour and liquid phase due

to cavitation is modelled by a Homogeneous Relaxation Model (HRM) (Bilicki and Kestin, 1990; Shields et al., 2011). The model assumes that the rate at which the instantaneous mass (x) approaches its equilibrium value (\bar{x}) depends on a time scale factor (θ) or relaxation factor. The linear relation is expressed as:

$$\frac{D_x}{Dt} = \frac{\bar{x} - x}{\theta}. \quad (20)$$

Two time scales are calculated, one for evaporation and another for condensation:

$$\theta_E = \theta_0 \alpha^{-0.54} \varphi^{-1.76}, \quad (21)$$

$$\theta_C = F \theta_0 \alpha^{-0.54} \varphi^{-1.76}. \quad (22)$$

237 Notice that α is the void fraction, equals to $(1 -$
 238 $\bar{Y})$. The value of θ_0 is set to $3.84e - 7s$ and φ is the
 239 non-dimensional pressure ratio.

$$\varphi = \frac{P_{sat} - P}{P_c - P_{sat}}, \quad (23)$$

where P_c denotes the critical pressure of the fluid. In equation 22, F has a value of 5000 according to the conclusions from previous analysis by He et al. (2017).

244 3. Methodology

245 The current study is divided in two steps. First,
 246 two existing injector nozzle geometries are used for
 247 the validation of the simulations in terms of the
 248 internal flow characteristics and the spray forma-
 249 tion processes. The internal flow is validated based
 250 on hydraulic data from a multi-hole nozzle, char-
 251 acterized by cylindrical orifices so that cavitation
 252 is induced. For the validation of the spray models,
 253 the so called "Spray A" from the Engine Combustion
 254 Network (ECN) ([https://ecn.sandia.gov/ecn-
 255 data-search/](https://ecn.sandia.gov/ecn-data-search/)), which is a single-hole conical nozzle,
 256 is selected. The advantage of this nozzle is that it is
 257 widely characterised in terms of the spray evolution
 258 by different experimental techniques.

259 Later on, the impact of the eccentricity in the
 260 outlet section of the nozzle is analysed. For this
 261 purpose, six different 3D nozzle geometries with in-
 262 creasing levels of eccentricity have been explored
 263 for this study (Table 1), using as a basis the geom-
 264 etry from a production 6-hole diesel nozzle. The
 265 initial dimensions of this injector were character-
 266 ized using silicone moulds. This method was widely

267 used in similar studies, providing a geometrical error 281
 268 error about 2% in the main nozzle magnitudes (Ma- 282
 269 cian et al., 2003; Payri et al., 2016, 2011; Salvador 283
 270 et al., 2018a,b). The whole internal geometry of the 284
 271 real injector, including the needle seat, sac, the hydro- 285
 272 griding radius and the outlet section, has been 286
 273 replicated for all the six elliptical nozzles. Even 287
 274 though the outlet area of the orifice remains constant, 288
 275 the nozzle shape varies as the minor radius 289
 276 (axial with respect to the injector body axis) de- 290
 277 creases and the major one (tangential to the in- 291
 278 jector) increases (see Figure 1a and 1b for further 292
 279 details). The outlet orifice has been defined taking 293
 280 into account the expressions below:

$$A_{ellipse} = \pi ab = D_{base}^2 \frac{\pi}{4} \mu m^2, \quad (24)$$

$$\text{being } a = \frac{A}{R_{min}\pi}, \quad (25)$$

$$\text{and } e = \frac{c}{a}. \quad (26)$$

Where a is the minor radius, b is the major radius 303
 and c is the so-called linear eccentricity:

$$c = \sqrt{a^2 - b^2}. \quad (27)$$

| Radius [μm] and eccentricities | | |
|---------------------------------------|---------------|------|
| R_{min} (b) | R_{max} (a) | e |
| 80 | 90.31 | 0.50 |
| 75 | 96.33 | 0.62 |
| 70 | 103.21 | 0.73 |
| 65 | 111.15 | 0.81 |
| 55 | 131.36 | 0.90 |
| 50 | 144.5 | 0.94 |

Table 1: Geometries used for the study.



(a) eccentricity = 0.50 (b) eccentricity = 0.94

Figure 1: 3D geometry models

In order to ensure the independence of the results 301
 from the computational boundaries, a $30 \times 30mm$ 302
 chamber domain has been chosen for the injection 303
 process (Figure 2). The symmetry of the problem 304
 allows to calculate a single 60° sector of the in- 305
 jector, corresponding to one nozzle orifice, reducing 306
 the computational effort. Turbulence is modelled 307
 by unsteady Reynolds-Averaged Navier-Stokes (U- 308
 RANS) methodology, employing a Favre-averaged 309
 formulation for compressible fluids. Given the high 310
 flow velocity and the expected appearance of cavi- 311
 tation, Reynolds values higher than 20000 have 312
 been estimated, so a turbulent flow is expected in- 313
 side the nozzle. For this reason, a standard $k - \epsilon$ 314
 model (Launder and Sharma, 1974; Launder and 315
 Spalding, 1974) has been selected as a turbulence 316
 model. Although this particular approach perfor- 317
 mance is known to be worse than others like the 318
 $k - \omega$ in recirculation zones (such as those gener- 319
 ated in cavitation problems) and low-Reynolds-number 320
 flows (David C. Wilcox, 1994), it has commonly pro- 321
 duced better results in free stream flow conditions 322
 (David C. Wilcox, 1994). The Re-Normalisation 323
 Group (RNG) $k - \epsilon$ (Yakhot and Smith, 1992) 324
 model was also proposed since it helps to overcome 325
 some of the numerical problems induced by separated 326
 flows. However, several studies using the $\Sigma - Y$ 327
 model found in literature use the standard $k - \epsilon$ 328
 model for similar purposes as the current study, with 329
 a modified value for the $C_{\epsilon 1}$ coefficient equals to 1.6 330
 instead of 1.44 (Dally et al., 1998; Garcia-Oliver 331
 et al., 2013; Hoyas et al., 2013; Janicka and Peters, 332
 1982; Pandal Blanco, 2016; Pope, 1978; Xue et al., 333
 2015). Therefore, this last configuration has been 334
 taken to ensure consistency with previous works. 335

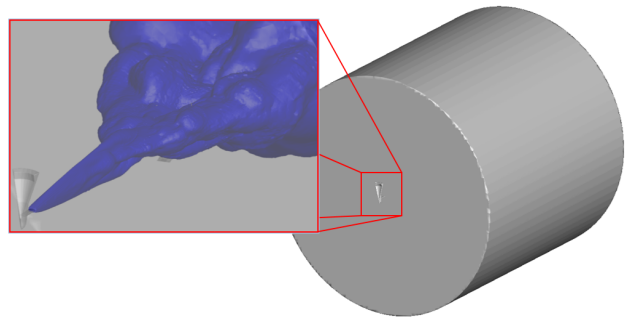


Figure 2: Simulated domain, $30 \times 30mm$

The energy equation has been solved in its inter- 336
 nal form. As already introduced, a Homogeneous 337
 Relaxation Model (HRM) (Bilicki et al., 1996; Bil- 338

319 icki and Kestin, 1990; Brusiani et al., 2013; Downar-
 320 Zapolski et al., 1996; Schmidt, 1997; Schmidt et al.,
 321 2010) has been chosen in order to solve the cavitation
 322 generated at the nozzle inlet in the multi-hole
 323 geometries. In this zone, the accelerating fuel de-
 324 taches from near walls and produces local pressure
 325 drops. This phenomenon depends on the injection
 326 pressure, the back-pressure and the nozzle geometry
 327 (Arcoumanis et al., 2000; López et al., 2017; Payri
 328 et al., 2005, 2004b; Salvador et al., 2015a, 2017; So-
 329 teriou et al., 2010; Sun et al., 2015). The geometries
 330 under study are expected to cavitate since none of
 331 them are conical. The effect of cavitation requires a
 332 small time step in order to reach convergence. This
 333 issue limits the total time of injection to 500 μs ,
 334 performed at full needle lift conditions.

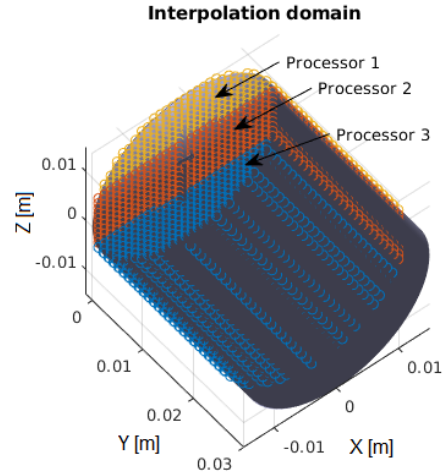
335 Regarding the boundary conditions, chamber
 336 outlet far boundaries (bottom circular plane and
 337 peripheral curved surface) are set as outflow con-
 338 ditions with zero normal gradient for the velocity.
 339 The inlet boundary at the nozzle has been defined
 340 in terms of a static pressure. A wall function has
 341 been applied to all wall boundaries. For reference
 342 nozzles, the injection parameters match the ECN
 343 target conditions ([https://ecn.sandia.gov/ecn-data-
 344 search/](https://ecn.sandia.gov/ecn-data-search/)) in non-evaporative experiments. On the
 345 other hand, the elliptical nozzles have been simu-
 346 lated at 200 MPa injection pressure and 3 MPa
 347 back-pressure, with an initial temperature of 303
 348 K. Table 2 summarizes all the applied conditions.

| Boundary conditions, $P[MPa]$, $T[K]$ | | | | |
|--|-----------|------------|-------|-------|
| Nozzles | P_{inj} | P_{back} | T_f | T_c |
| Spray A | 150 | 2 | 343 | 303 |
| Elliptical | 200 | 3 | 303 | 303 |

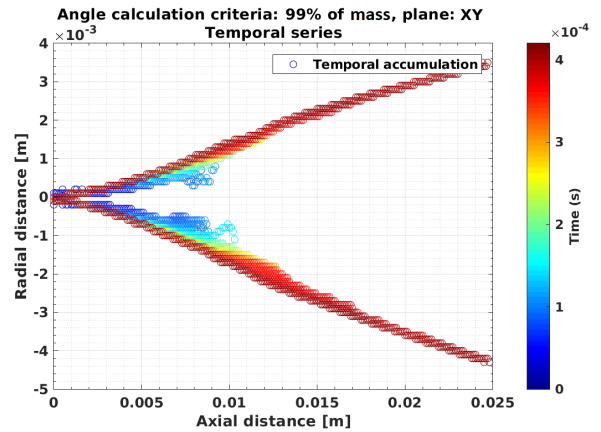
Table 2: CFD boundary conditions.

349 A transverse mass criteria has been chosen in order
 350 to calculate the angle. As the results produced
 351 by the software are provided in an *OctreeMesh*
 352 (Senecal et al., 2011), a Cartesian mesh with a 50
 353 μm resolution is generated and adjusted to the do-
 354 main for the first 20 mm (Figure 3a). Variables are
 355 then parallel interpolated for post-processing.

The transverse mass is then calculated according
 to the summation of the liquid mass in two planes
 projection XY (minor radius) and ZY (major ra-



(a) Angle calculation, virtual mesh generation.



(b) Points for CFD angle calculation, Spray A

Figure 3: CFD angle calculation methodology.

dius), (see Figure 3b).

$$m_{liquid} = \sum_{i=1}^n \bar{\rho}_i \tilde{Y}_{f_i} V_{mesh}. \quad (28)$$

356 Then, for each transverse integrated slice, the spray
 357 limits are calculated according to a certain percent-
 358 age in mass (95 or 99%) of the total mass contained
 359 in each axial slice.

360 Following the normalized path suggested by the
 361 ECN, N-dodecane fluid and vapour tabulated prop-
 362 erties have been used within the reference noz-
 363 zle simulations. Vapour and nitrogen have been
 364 treated as ideal and compressible gases, while N-
 365 dodecane is set as dependent on temperature and

366 pressure. With respect to the elliptical nozzles, a 400
 367 commercial diesel fuel has been chosen as working 401
 368 fluid and has also been characterized as a function 402
 369 of temperature and pressure. Temperature correla- 403
 370 tions have been implemented in a tabulated format 404
 371 while compressibility effect is taken into account 405
 372 by the compressibility modulus ($B = 1.49e9$ MPa). 406
 373 More details about how each of the main fuel prop- 407
 374 erties is considered and the literature works from 408
 375 which the information was extracted can be seen in 409
 376 Table 3.

| Property | Value or function |
|-------------------------|---|
| Density | $825.5\Delta e^{\frac{P-P_{ref}}{B}}$ [1] |
| Viscosity | $f(T, P_{ref})$ [1,2] |
| Vapour pressure | $f(T, P_{ref})$ [3] |
| Surface tension | $0.029N/m$ [4] |
| Specific heat (C_p) | $f(T, P_{ref})$ [3] |

1-Desantes et al. (2015)
 2-Salvador et al. (2018a)
 3-Kolev (2012)
 4-Dechoz and Rozé (2004)

Table 3: Diesel fuel main properties ($P_{ref} = 0.1$ MPa).

377 4. Model validation

378 Two kinds of validation have been performed in 413
 379 this study. On the one hand, coupled nozzle-spray 414
 380 model ($\Sigma - Y$) has been compared to an exten- 415
 381 sive dataset available in the literature for Spray 416
 382 A (injector #210675) from the Engine Combustion 417
 383 Network group ([https://ecn.sandia.gov/ecn-](https://ecn.sandia.gov/ecn-data-search/) 418
 384 [data search/](https://ecn.sandia.gov/ecn-data-search/)), which represents a conical (non- 419
 385 cavitating, HRM model not included) single-hole 420
 386 and almost axi-symmetric geometry. On the other 421
 387 hand, a partial validation of the injection process 422
 388 with cavitation has been performed based on noz- 423
 389 zle internal flow experimental data for a cylindri- 424
 390 cal multi-hole nozzle, whose internal geometry and 425
 391 inner flow parameters have been previously char- 426
 392 acterised. All the models listed above have been 427
 393 configured within the software CONVERGE CFD 428
 394 (<https://convergecf.com>).

395 Validation of single-hole Spray A

396 Figure 4a shows the geometry of the Spray A noz- 432
 397 zle, which as previous said represents a single- 433
 398 hole quasi-axi-symmetric layout with a slight devi- 434
 399 ation of the nozzle from the main jector body axis. 435

Since this deviation barely affects the spray perfor-
 mance, it is commonly considered axi-symmetric.
 The 3D geometry has been acquired from the *x-ray*
 measurements provided in the ECN data base
 (Kastengren et al., 2012). The nominal diameter
 is measured at $90 \mu m$ and the nozzle exhibits a
k-factor of 1.5 (Macian et al., 2003).

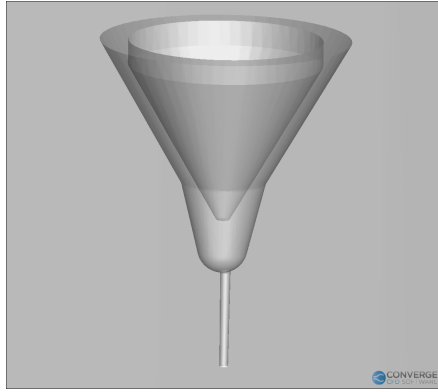
The chosen mesh configuration provides a mini-
 mum of fifteen rows of cells inside the nozzle, rep-
 resenting an average of $6 \mu m$. Some authors have
 established a minimum of ten cells as a good ap-
 proach (Garcia-Oliver et al., 2013; Lebas et al.;
 Xue et al., 2015).

| Cell size [μm] | |
|-----------------------|-----------------|
| Mesh region | Spray A |
| Base size | 384 |
| Nozzle | 6 |
| Near nozzle spray | 12 (up to 5 mm) |
| Needle | 48 |
| AMR u (nozzle) | Disabled |
| AMR α (nozzle) | Disabled |
| AMR u (spray) | 24 |
| Total cells | $\sim 9e6$ |

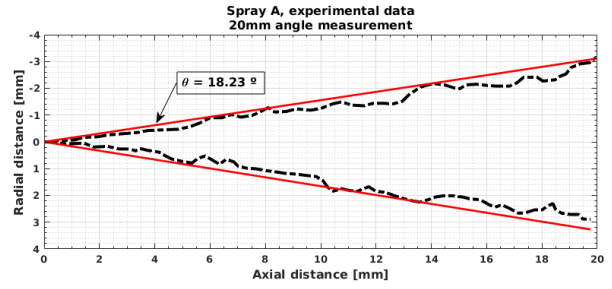
Table 4: Mesh configuration for Spray A

Figures 4b and 4c show the computational mass
 flow and momentum flux at the nozzle outlet to-
 gether with the experimental ones, extracted from
 the literature (Pickett et al., 2011, 2013). Despite
 the experimental data is obtained from a transient
 injection process, while the simulations are made
 at steady maximum needle lift, it can be noted
 that a good agreement between steady-state parts
 of the injection is reached for either mass flow rate
 (Figure 4b) or momentum flux (Figure 4c).

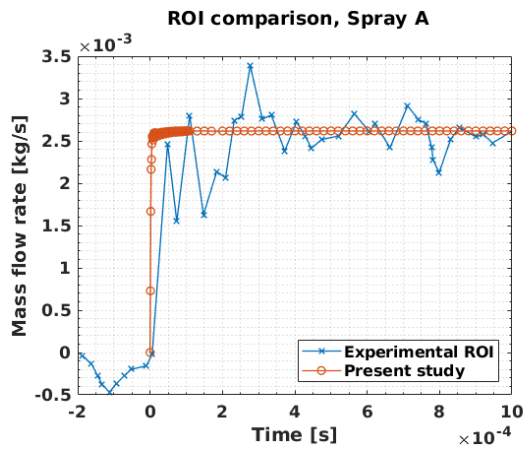
The spray angle calculation has been carried out
 following the methodology in section 2, computing
 an average angle of 19.1° for the 99% of the pro-
 jected radial mass and 14.6° for the 95% in mass
 (Figure 5b). The interpolation of the angle has
 been conducted over the first 20 mm of the simu-
 lation discharge chamber. Mean angle values were
 calculated over the steady part of the simulation
 ($> 300 \mu s$). The experimental angle data is avail-
 able in previous works (Pickett et al., 2011, 2013)
 based on Diffused Back-Light (DBI) visualisation
 tests. Figure 5a shows the fitting lines for an ex-
 perimental angle up to 20 mm axial distance from



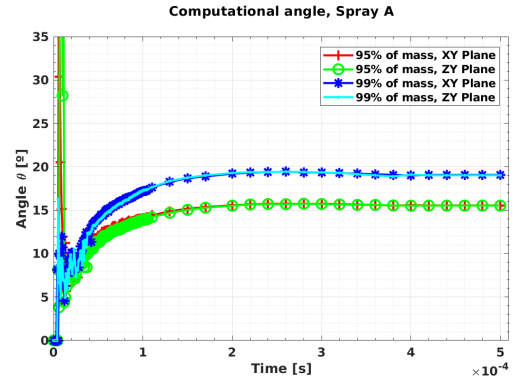
(a) Spray A, 3D geometry



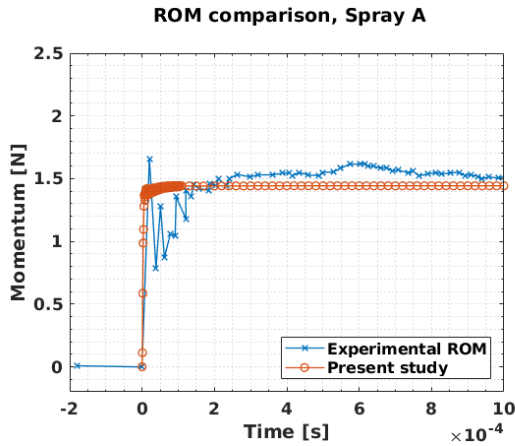
(a) Spray A, experimental angle (Pickett et al., 2013) contour and fitting lines. A DBI technique was used for measuring the angle at 22.3 kg/m^3 of discharge density and 150 MPa injection pressure.



(b) Rate of injection



(b) Spray A, computational angle.



(c) Rate of momentum

Figure 4: Mass flow and momentum comparison for Spray A nozzle.

436 the nozzle.

437 Taking into account the experimental data, an ab-

Figure 5: Spray A results.

438 solute error of 0.87° is found in the spray angle.

439 X-ray radiography technology applied to the study of the injection process (Duke et al., 2017; Kastengren et al., 2009, 2014, 2012) allows a deeper look inside the spray microscopic behaviour. Comparisons in projected mass density are provided below. Figure 6 shows several Gaussian profiles of projected mass density (PMD) along the spray axis (at 0.1 mm, 2 mm, 4 mm, 6 mm distance) on the XY plane. Although the Spray A injector is considered to be quasi-axi-symmetric, the slight deviation of the nozzle from the main injector body axis (Pickett et al., 2014) is captured by the deviation from 0 of the XY projection (Figure 6a, 6b, 6c, 6d). As reported in similar studies (Desantes et al., 2016b; Xue et al., 2015), even if the PMD is well captured along first millimetres of the spray, the CFD case shows higher values far from the nozzle exit. Beyond 6 mm, the de-

457 cay of the projected mass density is severe, and 508
 458 the difference between experiments and simula- 509
 459 tion significantly grows. Similar conclusions can 510
 460 be obtained looking at 2-dimensional PMD con- 511
 461 tours available in Figures 7a and 7b. As it can
 462 be seen, the simulation provides a faster axial de- 512
 463 cay and a wider radial evolution of PMD com-
 464 pared to the experimental reference data as the 513
 465 spray develops far from the nozzle exit. Advanced
 466 turbulence approaches such as Large Eddy Sim-
 467 ulation (LES), coupled with capturing interface
 468 methods, have shown to better describe the evo-
 469 lution of the projected mass density in literature
 470 studies, as reported in the literature (Anez et al.,
 471 2018; Desantes et al., 2017). However, since the
 472 main objective of the current study is to analyse
 473 the impact of the elliptical orifices on the nozzle
 474 flow behaviour and the primary atomization, the
 475 numerical setup used is deemed appropriate, since
 476 it has shown to be capable to properly capture
 477 the spray behaviour in the first millimetres of the
 478 nozzle outlet at a reduced computational cost.

479 Finally, a self similarity study for the velocity dis-
 480 tribution has been performed. Figure 8 shows
 481 the evolution of the inverse of the velocity in the
 482 spray axis divided by the velocity at the nozzle
 483 orifice outlet. Additionally, the axial position has
 484 been made non-dimensional with respect to the
 485 nozzle equivalent diameter. As it can be seen,
 486 there is a linear increase after the so called intact
 487 length, as it would be predicted by gas jet theory.
 488 The results have an almost perfect match with
 489 the same information extracted from the work by
 490 Taub et al. (2013) based on Direct Numerical Sim-
 491 ulations. The slope of this increase has been com-
 492 puted by doing a linear fit to the data extracted
 493 from the simulations and compared with experi-
 494 mental data from Hussein et al. (1994), showing a
 495 difference of approximately 4%. Both results can
 496 be seen as a further validation of the capability of
 497 the current model to properly capture the physics
 498 related with the momentum exchange between the
 499 fuel spray and the environment.

500 The previously mentioned result is complemented
 501 with the analysis of the radial distribution of the
 502 non-dimensional velocity, depicted in Figure 9.
 503 For axial positions equal or further than 24 times
 504 the equivalent diameter, all the radial profiles ex-
 505 pressed in terms of the ratio between radial and
 506 axial positions collapse into a single curve. This
 507 corresponds to the disperse region of the spray,

whose behaviour can be predicted according to gas
 jet theory. Instead, for closer positions to the noz-
 zle tip a slight variation of this profile can be ob-
 served.

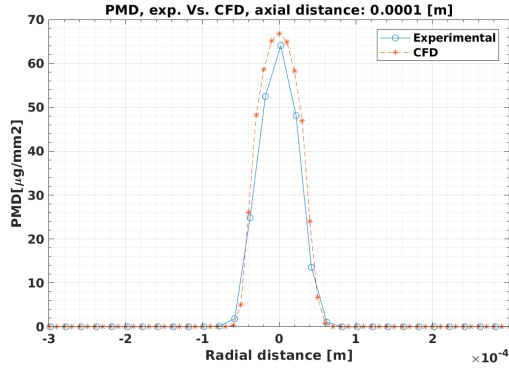
Multi-hole reference cylindrical nozzle

513 The second part of the model validation is focused
 514 on the analysis of the internal flow under cavitat-
 515 ing conditions. Here, the mentioned 3D geome-
 516 try of a commercial 6 holes injector with cylin-
 517 drical orifices, previously characterised experimen-
 518 tally from an hydraulic standpoint (Salvador et al.,
 519 2011), is used. All simulations are performed with
 520 the same physical models already described for the
 521 spray A case, and have been run until a steady
 522 state flow was reached. Since cavitation is ex-
 523 pected, the HRM model has been incorporated
 524 to the model equations. In a preliminary step,
 525 a mesh independence study was completed using
 526 three different levels of refinement, with an incre-
 527 ment of 2^n size ratio for the nozzle region, as es-
 528 tablished in Table 5. Additionally, the Adaptive
 529 Mesh Refinement (AMR) method is activated for
 530 subgrid velocity levels higher than 1 m/s and 0.1
 531 of void fraction.

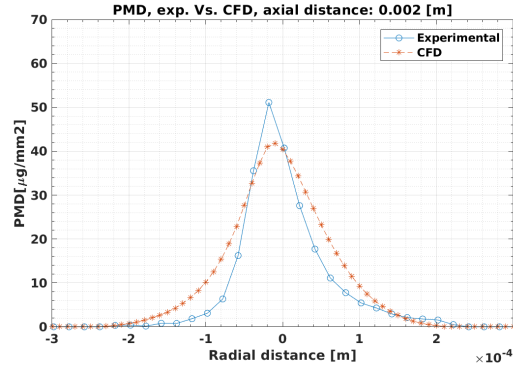
| Mesh independence study | | | |
|-------------------------|----------------------|-------|--------|
| Base size = 384 μm | Refinement level n | | |
| Region | L | M | H |
| Nozzle | 2 | 3 | 4 |
| Nozzle wall (3 levels) | 5 | 6 | 7 |
| AMR velocity | 3 | 4 | 5 |
| AMR void fraction | 4 | 5 | 6 |
| Needle | 2 | 3 | 3 |
| Total elements | 18247 | 85687 | 389148 |

Table 5: Mesh configuration for the six orifices nozzle.

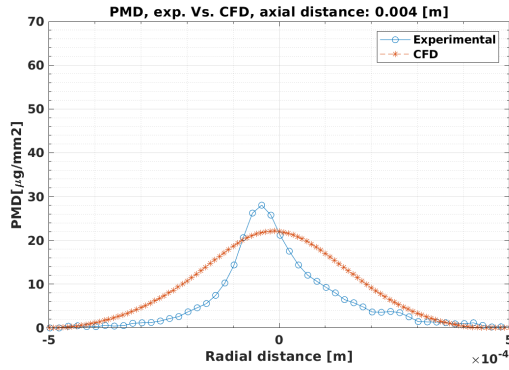
532 Mass flow rate and vapour mass at the out-
 533 let have been selected as the reference param-
 534 eters for analysing the grid convergence. Once a
 535 steady state value of the selected variables has
 536 been reached, the convergence of the mesh was
 537 checked as described in Roache (1994) and Sal-
 538 vador et al. (2018a). The small committed error
 539 between the results and the Richardson extrap-
 540 olation ($P_{rh} < 0.47\%$), and the very low grid con-
 541 vergence index (GCI) leads to conclude that these
 542 variables are located into the asymptotic zone of



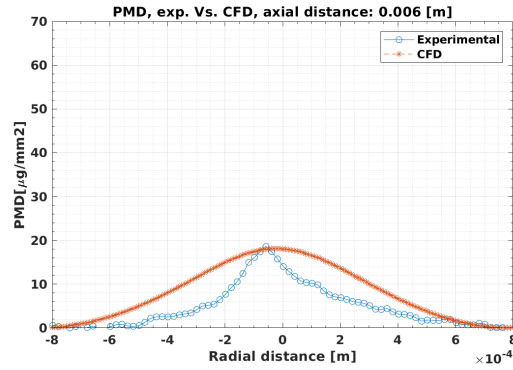
(a) Radial PMD, axial distance: 0.1 mm



(b) Radial PMD, axial distance: 2 mm



(c) Radial PMD, axial distance: 4 mm



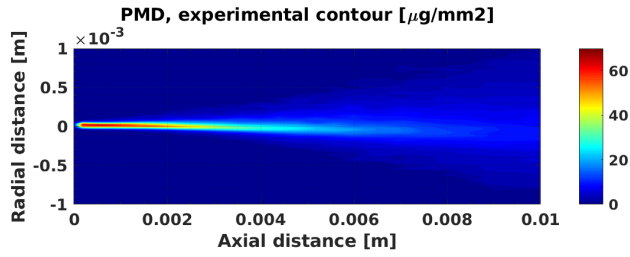
(d) Radial PMD, axial distance: 6 mm

Figure 6: Projected mass density profiles on the XY plane, Spray A.

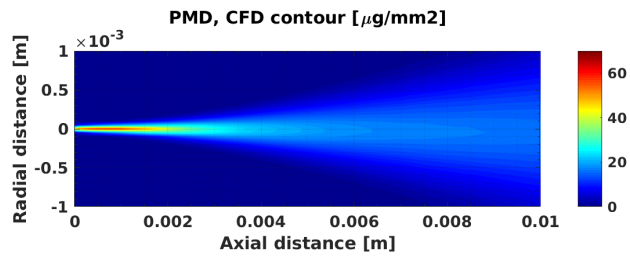
543 its mesh dependent curves with a mesh conver- 561
 544 gence order of 2. The GCI slightly varies between 562
 545 the low and medium mesh resolution (0.0021 and 563
 546 0.0058 for mass flow and vapour mass, respec- 564
 547 tively) and the medium to high resolution step 565
 548 (0.0086 and 0.0012 for mass flow and vapour mass, 566
 549 respectively). It was then deemed valid due to 567
 550 the low values achieved. However, for the simu- 568
 551 lations ahead the configuration with the highest 569
 552 mesh refinement has been chosen for the internal 570
 553 flow. The decision was based on the importance of 571
 554 not only reproduce the mean value of the flow, but 572
 555 also the particular distribution of the velocity and 573
 556 vapour profiles at the nozzle outlet. Furthermore, 574
 557 the AMR performance can be greatly conditioned 575
 558 by the initial grid size as studied in Payri et al. 576
 559 (2019). A superior surface refinement ensures the 577
 560 stability of the calculations when cavitation ap-

561 pears, and the correct generation of a initial gra-
 562 dent for the AMR void fraction subgrid. It has
 563 to be noticed that for the nozzle with the high-
 564 est eccentricity the resultant minor radius has 50
 565 μm length. The cell size must take into account
 566 this reduction of the aspect ratio and provide a
 567 suitable number of elements inside the orifice.

568 The experimental validation of the flow was car-
 569 ried out by means of several mass flow rate mea-
 570 surements at three injection pressures and six
 571 back-pressures (Salvador et al., 2011). Figure 11
 572 depicts the values for the CFD and experimental
 573 results. As appreciated, the code is able to prop-
 574 erly reproduce the mass flow choking conditions
 575 (the point at which mass flow rate reaches a crit-
 576 ical limit value). An error of 5.4% is found for
 577 the maximum injection pressure of 160 MPa. The
 578 error is expected to progressively decrease as the



(a) Projected mass density in 2D view, X-Ray data from the Spray A.



(b) Projected mass density in 2D view, CFD post-processed simulation from the Spray A.

Figure 7: Projected mass density contours, Spray A. Experimental data extracted from <https://ecn.sandia.gov/rad675/> and reported in Kastengren et al. (2014)

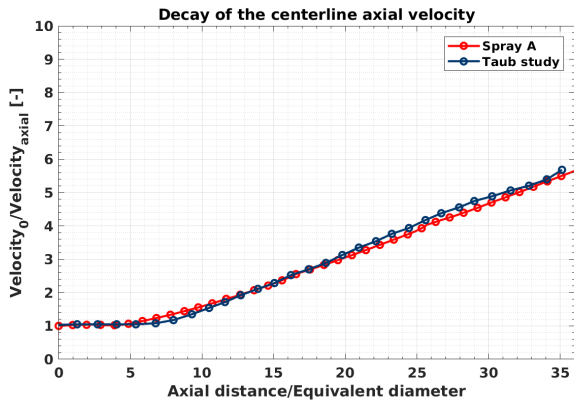


Figure 8: Axial evolution of the inverse of the non-dimensional velocity at the spray centerline.

579 injection pressure magnitude increases.

580 5. Results and discussion

581 A first sight to the effect of the eccentricity in
 582 the injection nozzle is carried out by the study of
 583 the inner flow. For this purpose, the main non-

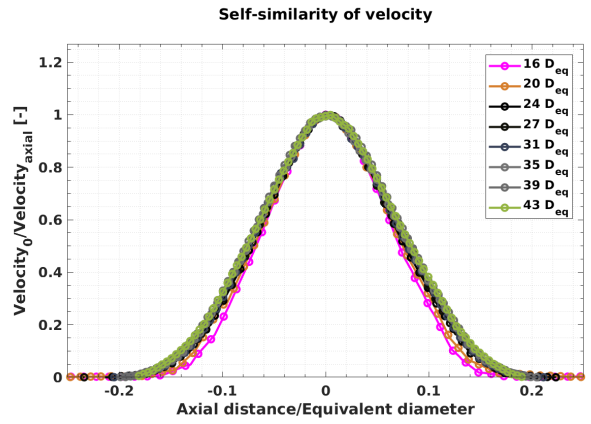


Figure 9: Radial distribution of the non-dimensional velocity

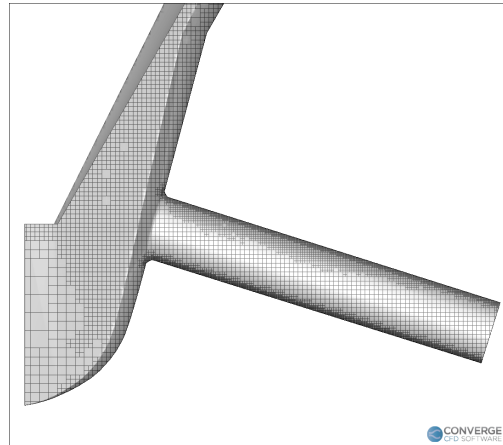


Figure 10: Detail of mesh configuration.

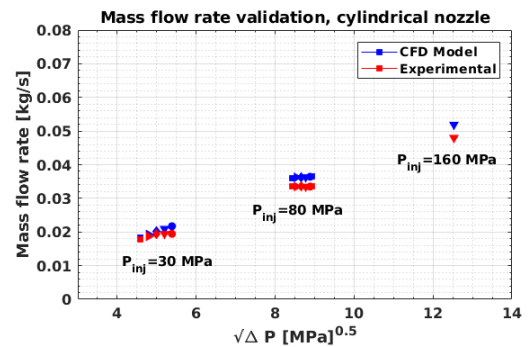


Figure 11: Experimental vs. Computational mass flow. Each symbol represents a different back pressure from 0.1 to 9 MPa.

584 dimensional flow coefficients of the nozzle, mainly 628
 585 including the discharge coefficient C_d , the velocity 629
 586 coefficient C_v and the area coefficient C_a , have been 630
 587 obtained (Salvador et al., 2015a). The discharge 631
 588 coefficient, C_d , has been calculated according to the 632
 589 ideal mass flow value based on Bernoulli's equation: 633

$$C_d = \frac{\dot{m}_f}{\rho_l A_0 u_{th}} = \frac{\dot{m}_f}{A_0 \sqrt{2\rho_l \Delta P}} \quad , \quad (29) \quad 634$$

590 where \dot{m}_f is the mass flow, ρ_l is the liquid density, 637
 591 A_0 is the geometric outlet orifice area and ΔP is 638
 592 the pressure drop. 639

From the comparison of the nozzle effective vs. 640
 theoretical velocities, the velocity coefficient is cal- 641
 culated as: 642

$$C_v = \frac{u_{eff}}{u_{th}}. \quad (30) \quad 643$$

593 Finally, the area coefficient can be calculated tak- 645
 594 ing into account that the relationship $C_d = C_v C_a$. 646
 595 647

596 Figure 12 shows the flow parameters from the el- 648
 597 liptical nozzles calculations. As it can be seen, mass 649
 598 flow rate slightly rises its value as the eccentricity 650
 599 increases, while the momentum value remains al- 651
 600 most unchanged. In the studies by Lee et al. (2006) 652
 601 and Ku et al. (2011), a similar behaviour was ob- 653
 602 served for the mass flow. It is also in agreement 654
 603 with a previous publication by the authors (Molina 655
 604 et al., 2014). The higher mass flow and similar out- 656
 605 let momentum are a consequence of a decreasing 657
 606 trend in the effective outlet velocity with increas- 658
 607 ing eccentricity, which can be explained by the in- 659
 608 teraction between the eccentricity and the intensity 660
 609 of cavitation. The internal flow parameters (Figure 661
 610 12) show that cavitation is reduced as the eccen- 662
 611 tricity increases. Less cavitation produces a greater 663
 612 area coefficient, as it can be seen from the figure, 664
 613 but a lower velocity coefficient (Payri et al., 2005). 665
 614 In terms of mass flow, an increase would be foreseen 666
 615 when increasing the eccentricity, since the higher 667
 616 C_a would induce an also higher C_d if the velocity 668
 617 remained constant. However, since the velocity is 669
 618 also reduced when eccentricity diminishes, two op- 670
 619 posing effects are found, preventing the mass flow 671
 620 rate and momentum from suffering major changes. 672

621 According to the literature, more intense cavit- 673
 622 ation field induces a slightly higher momentum (sim- 674
 623 ilar mass flow, higher velocity), which would en- 675
 624 force the spread angle and mixing process (Chaves 676
 625 et al., 1995; Payri et al., 2004a; Tamaki et al., 2001). 677
 626 Additionally, many previous works available in the 678
 627 literature (Hiroyasu and Miao, 2003; Naber and 679

Siebers, 1996) show the spray penetration can be 628
 mostly linked to the spray momentum and spread- 629
 ing angle. Therefore, slightly larger spray penetra- 630
 tion could be anticipated for the cylindrical noz- 631
 zles, which are characterized by slightly larger mo- 632
 mentum. However, the following paragraphs will 633
 demonstrate that the sole study of the average flow 634
 parameters at the nozzle outlet is not enough to 635
 account the influence of eccentricity in the spray 636
 performance. 637

First of all, not only the cavitation intensity 638
 but its distribution along the nozzle section needs 639
 to be considered. As it can be seen from Figure 640
 13, although the intensity of the void fraction 641
 is higher in the nozzle with $e = 0.50$ (left side), 642
 the distribution of vapour in the most elliptical 643
 nozzle is wider over the whole section (right side). 644
 Even if the generation of vapour inside the nozzle 645
 is well known to improve the atomization from 646
 the literature, the low amount of experimental 647
 measurements from inside the nozzle hardens 648
 the complete understanding of how the vapour 649
 distribution itself affects the phenomena involved. 650
 As it could be anticipated, the aspect ratio of the 651
 elliptical nozzles (i.e. the ratio between major 652
 and minor radii) affects the vapour distribution 653
 field, in particular the interaction between the 654
 bottom and top side vapour in the nozzle outlet. 655
 Figures 13a and 13b show how the stream-lines are 656
 then approaching each other along the nozzle as 657
 eccentricity increases, which supports this effect. 658
 Hong et al. (2010) suggested that the cavitation 659
 should be improved in the cross sectional area of 660
 the elliptical nozzles because of a severe contrac- 661
 tion of the stream-lines. However, this statement 662
 may not be applied to multi-hole configurations, 663
 since the stream-lines are not symmetric. Unlike 664
 single-hole nozzles, in the proposed geometries 665
 the vapour is generated mainly in the top-part of 666
 the cross-section. This section, where the fluid 667
 accelerates, is wider for the nozzles with higher 668
 aspect ratio, and allows a larger path for the most 669
 critical stream-lines. A larger local curvature dis- 670
 tributes the stream flow and reduces the pressure 671
 drop, so the vapour peak is lower. Additionally, 672
 it enforces the distribution of the vapour over the 673
 whole section, as it was already seen in Figure 13. 674
 Furthermore, the higher perimeter of the ellipse 675
 provides a more significant interaction of the spray 676
 section with the chamber gas. With respect to the 677
 thermodynamic properties of the fluid, no major 678
 differences have been identified. 679

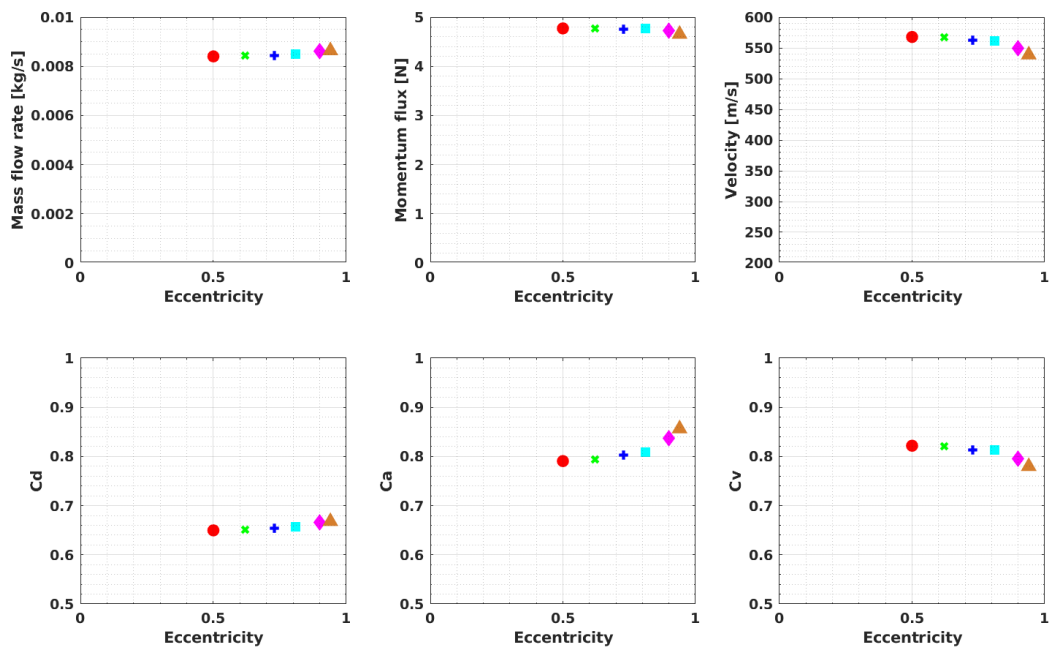


Figure 12: Hydraulic characterization of the elliptical nozzles. The principal coefficients and variables have been calculated at the outlet for each nozzle. It includes the mass flow and momentum flux, effective velocity and non-dimensional parameters: the discharge coefficient, C_d , area coefficient, C_a , and velocity coefficient, C_v .

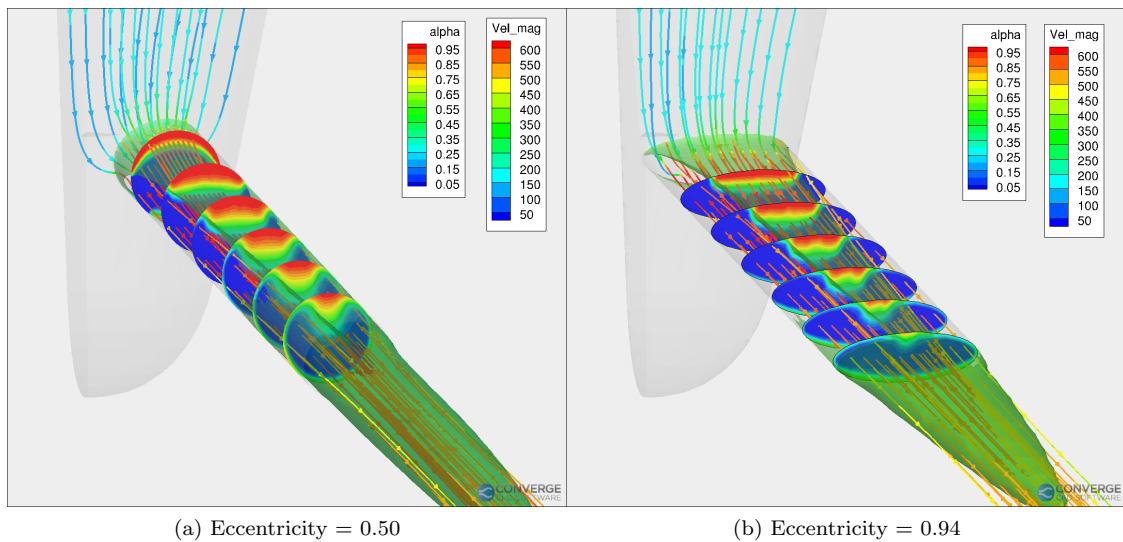


Figure 13: Flow conditions along the nozzle: the coloured stream-lines represent the variation of the velocity magnitude along the nozzle, while the radial slices show the void fraction evolution in six equally spaced sections. The iso-volume in green represents the void fraction for a value of 0.5. Notice how the vapour spreads further away from the orifice for the nozzle with lower eccentricity.

680
681

One important parameter that can be evaluated

682

683

to start analysing the impact of the eccentricity in spray development is the evolution of the mixing

684 field. This information is depicted in terms of the 732
 685 axial distribution of the fuel mass fraction (Figure 733
 686 14), as well as the radial distribution of the fuel 734
 687 mass fraction at four axial positions and for two
 688 different planes (XY and ZY) in Figures 15a-15h.
 689 The axial distribution is defines in terms of the axial
 690 location divided by the equivalent diameter, defined
 691 as:

$$D_{eq} = D_o \sqrt{\frac{\rho_f}{\rho_a}} \quad (31)$$

692 where D_o is the diameter of a circle that would
 693 produce the same section as the outlet orifice of the
 694 eccentric nozzles, ρ_f the liquid fuel density and ρ_a
 695 the air density in the discharge chamber.

696 In the near nozzle region (up to 3 mm or 3.5
 697 equivalent diameters), the axial evolution is very
 698 similar for all nozzles, while the radial distribution
 699 results are directly influenced by the nozzle mor-
 700 phology (Figure 15a and 15b). As the spray pen-
 701 etrates inside the chamber (3-8 mm, 3.5-9 equiv- 735
 702 alent diameters), the axial evolution is still similar, 736
 703 and the radial limits for the mass fraction start 737
 704 to become also more similar for both planes (Fig- 738
 705 ure 15c and 15d). Beyond 8 mm (approximately 739
 706 9 equivalent diameters), the axial evolution starts 740
 707 to be affected by the nozzle eccentricity, which can 741
 708 be also seen in the fact that the radial profiles as- 742
 709 sociated to the more elliptical nozzles seem to re- 743
 710 duce their fraction peak in favour of a wider curve 744
 711 (Figure 15e and 15f). A decreasing value of the 745
 712 liquid mass fraction peak can only take place if 746
 713 the equivalent quantity of liquid is radially scat- 747
 714 tered, that is, the angle of the spray is also big- 748
 715 ger. An inversion of width between both XY and 749
 716 ZY planes (corresponding to the minor and major 750
 717 axis, respectively) appears before reaching the 751
 718 12 mm (approximately 14 equivalent diameters) po- 752
 719 sition. This phenomenon becomes more severe as the 753
 720 aspect ratio increases (Figures 15g and 15h). Sim- 754
 721 ilar behaviour has been found by Yu et al. (Yu 755
 722 et al., 2018) in cavitating single-hole nozzles. In 756
 723 that case, where the flow enters symmetrically (in 757
 724 the direction of the nozzle axis), the initial pertur- 758
 725 bation starts on the sides of the major axis due to 759
 726 a greater contraction of the stream-lines. This pro- 760
 727 duces an initial larger dispersion in the ZY (major 761
 728 axis) plane (Hong et al., 2010). In the case of the 762
 729 present study, cavitation is generated in the top and 763
 730 bottom sections of the minor axis as a result of the 764
 731 inclination angle of the nozzle orifice with respect 765

to the injector axis (Salvador et al., 2015a). Hence,
 a wider spreading angle would be expected for the
 XY plane.

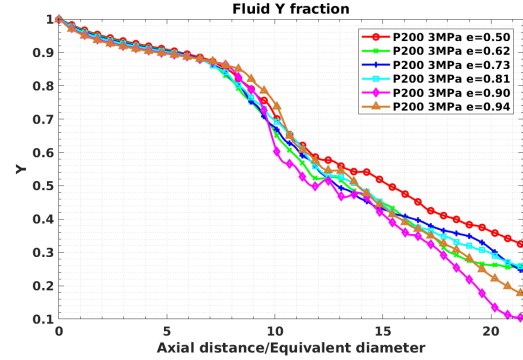


Figure 14: Axial liquid mass fraction

The radial and axial velocity profiles have also
 been extracted. The tendencies are similar to those
 of the liquid fuel mass fraction. A primary influence
 of the outlet geometry is followed by an almost per-
 fect matching in the maximum value and shape of
 the velocity profiles as the spray develops in axial
 direction (Figures 16a, 16b, 16c, 16d). For an in-
 termediate point (8 mm, 9 equivalent diameters),
 the velocity starts to decrease faster for higher ec-
 centricity values (Figures 16e, 16f, 16g and 16h).
 A faster dispersion of the fuel over the chamber is
 consistent with an earlier velocity fall. The mass
 exchange between the injected liquid and the inert
 gas (because of turbulent friction) results in kinetic
 energy losses which are, in fact, velocity losses. A
 similar trend can be seen in Figure 17 looking at
 the evolution of the inverse of the centerline veloc-
 ity divided by the outlet velocity. While in the case
 of a circular nozzle (i.e. symmetric jet) a linear
 trend would be seen, as it was already analyzed for
 Spray A data in Figure 8, for the elliptical geome-
 tries this linear trend can only be perceived for an
 axial distance up to 10 times the equivalent diam-
 eter. From that point on, inverse of the velocity
 clearly increases with a faster rate than a linear
 trend, actually more intense as the nozzle eccen-
 tricity increases.

Figure 18 represents the air entrainment for each
 nozzle spray. As it can be seen, there is a general
 trend of increasing entrainment as the eccentricity
 rises. A smooth growing trend is observed for the

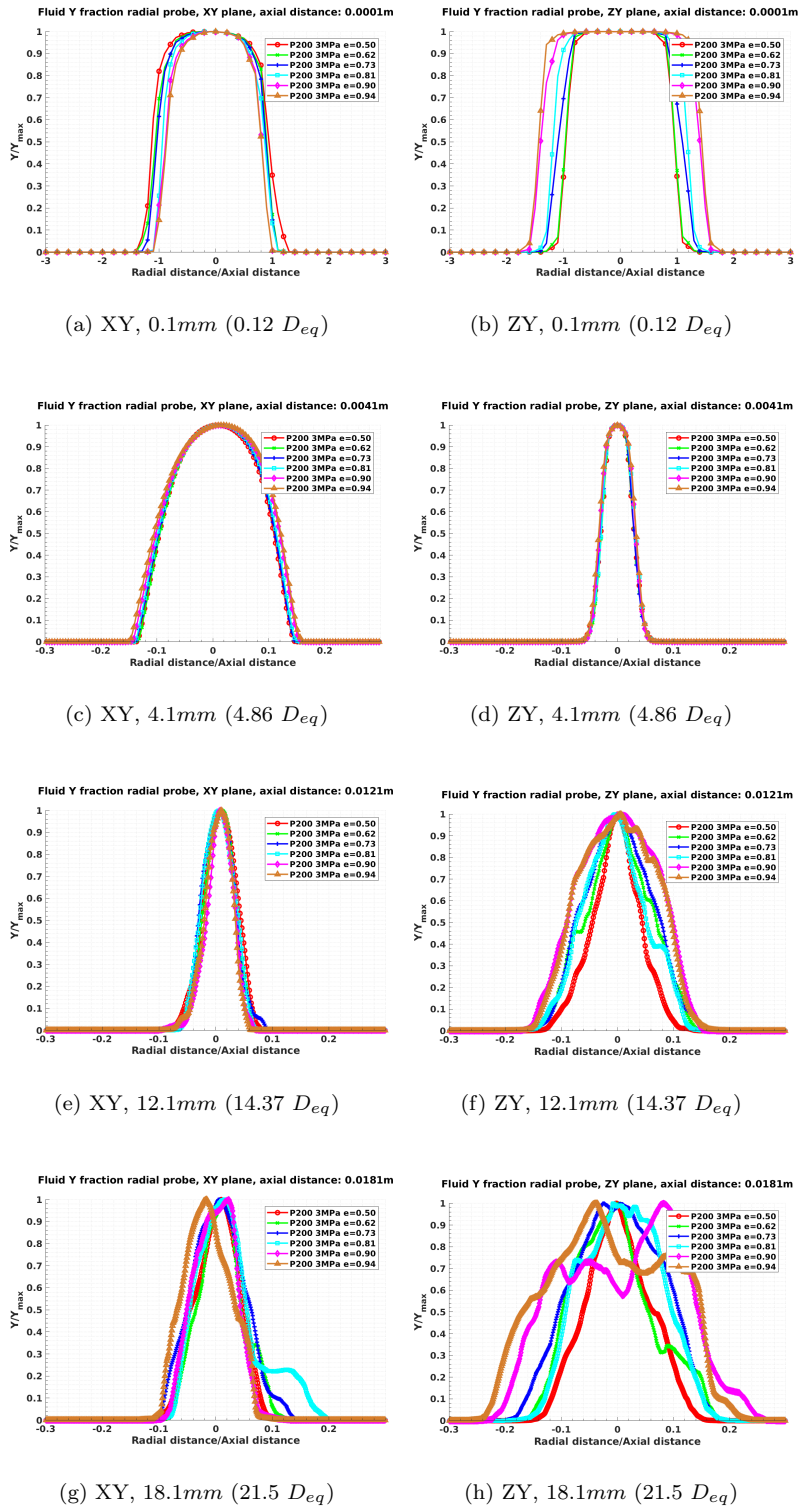


Figure 15: Radial liquid mass fraction profiles for the elliptical nozzles.

766 first four nozzles ($e = 0.50 \div 0.81$) while the two 808
767 last cases are characterised by a bigger initial 809
768 entrainment. In line with the discussion above, the 810
769 enhanced air entrainment is consistent with a wider 811
770 divergence of the angle and a slightly bigger mass 812
771 flow rate (Figure 12) (Araneo et al., 1999; Mac- 813
772 Gregor, 1991). Both liquid fuel mass fraction and 814
773 velocity profiles indicate that the spreading angle 815
774 in ZY plane is enhanced as the eccentricity of the 816
775 nozzle increases. Taking this into account, its im- 817
776 pact on the spray penetration can be evaluated. In 818
777 this sense, if the spray momentum is defined as:

$$\dot{M}(x) = \dot{M}_0 = \dot{m}_f U_0 = \int_A \rho_f U^2(x) dA. \quad (32)$$

The relationship between the spreading angle and the penetration can be established as follows (Desantes et al., 2006):

$$S(t) \propto M_f^{0.25} \rho_a^{-0.25} \tan^{-0.5}(\theta/2) t^{0.5}. \quad (33)$$

778 The penetration is then proportional to the mo- 830
779 mentum and inversely proportional to the tangent 831
780 of the spreading angle. From Figure 14, it can be 832
781 observed how beyond a medium distance from the 833
782 nozzle outlet, the elliptical nozzles diminish the li- 834
783 quid fraction faster along the injection axis, which 835
784 must be supported by an increment of the spread- 836
785 ing angle. Given that the momentum (12) does not 837
786 change significantly, an angle reduction will cause a 838
787 slower penetration slope. From a qualitative view, 839
788 Figure 19 shows how the 0.01 mass fraction iso- 840
789 volume regions for the most extreme nozzles (al- 841
790 most cylindrical and very elliptical), highlighting 842
791 the wider dispersion from the most eccentric nozzle 843
792 as the spray develops. 844

793 Even if the momentum value is nearly the same 845
794 for all nozzles, the interaction of this momentum 846
795 with the ambient gas is not. On the one hand, the 847
796 surface of elliptical nozzles adds an extra perimeter 848
797 of contact with the air for a same geometric area 849
798 value. On the other hand, the momentum thickness 850
799 (Krothapalli et al., 1981) varies across the section 851
800 in different ways for all cases so a lineal behaviour is 852
801 not necessarily expected between the sprays. This 853
802 surface interaction gain between the discharge gas 854
803 and the diesel jet is exponentially increasing with 855
804 eccentricity. From Figure 20, the numerical breach 856
805 in the shape area interaction between the first four 857
806 nozzles ($e = 0.50 \div 0.81$) and the two last nozzles 858
807 ($e = 0.90$ and 0.94) can provide some explanation 859

to the leap in entrainment. The resulting jet shape at the outlet for the maximum accounted eccentricity originates a value of 21.27% over the initial cylindrical nozzle perimeter for the same geometric area. This fact makes the rise in surface interaction compatible in general terms with the results for the entrainment and angle.

Finally, Figures 21a and 21b show the average computed angle (section 3) for all the elliptical nozzles. The angle projected on XY plane (21a) oscillates around 14° with no clear trend. The deviation from the mean value (dotted grey line) does not exceed 1.5° . From what was exposed in the internal flow parameters, the more cylindrical nozzle should develop a higher XY angle due to a more intense cavitation. However, the decreasing thickness in that plane for the elliptical nozzles also favours the increment of the angle due to instabilities. These effects oppose each other and may be the cause of an almost constant XY angle. This behaviour can be also connected to the fluctuations produced by cavitation, given that it takes place in the top and bottom parts of the nozzle section (minor axis view, XY plane).

The pulsatile and unsteady instabilities of vapour could lead to a still transient deposition of liquid in the XY plane for the simulated time. Nevertheless, this result is in agreement with the mass fraction profiles in the radial XY plane (Figure 15e, 15g), where the limit threshold value of the mass fraction appears in almost the same radial coordinate. Differently, the angle on ZY projection depicted in Figure 21b shows a clear tendency also according to the right column of picture 15, indicating that the divergence of the angle in ZY is proportional to the eccentricity value. Continuing with the pattern previously suggested in the entrainment discussion, a smooth jump in the angle is found until a eccentricity value of 0.81 while the last two nozzles shows a wider but closer angle. Regarding the angle proximity between nozzles 5 and 6, the proposed simulations may have reached the eccentricity threshold value at which the spray angle no longer increases. An increment about 10° is detected for the maximum eccentricity nozzle with respect to the lower one. Hong et al. (2010) showed in its experiments with transparent nozzles how the angle increases in both major and minor axis planes when elliptical single-hole nozzles are subjected to cavitation. However, in those proposed geometries, the cavitation and hence the source of instabilities were located in the major axis extremes, the opposite to

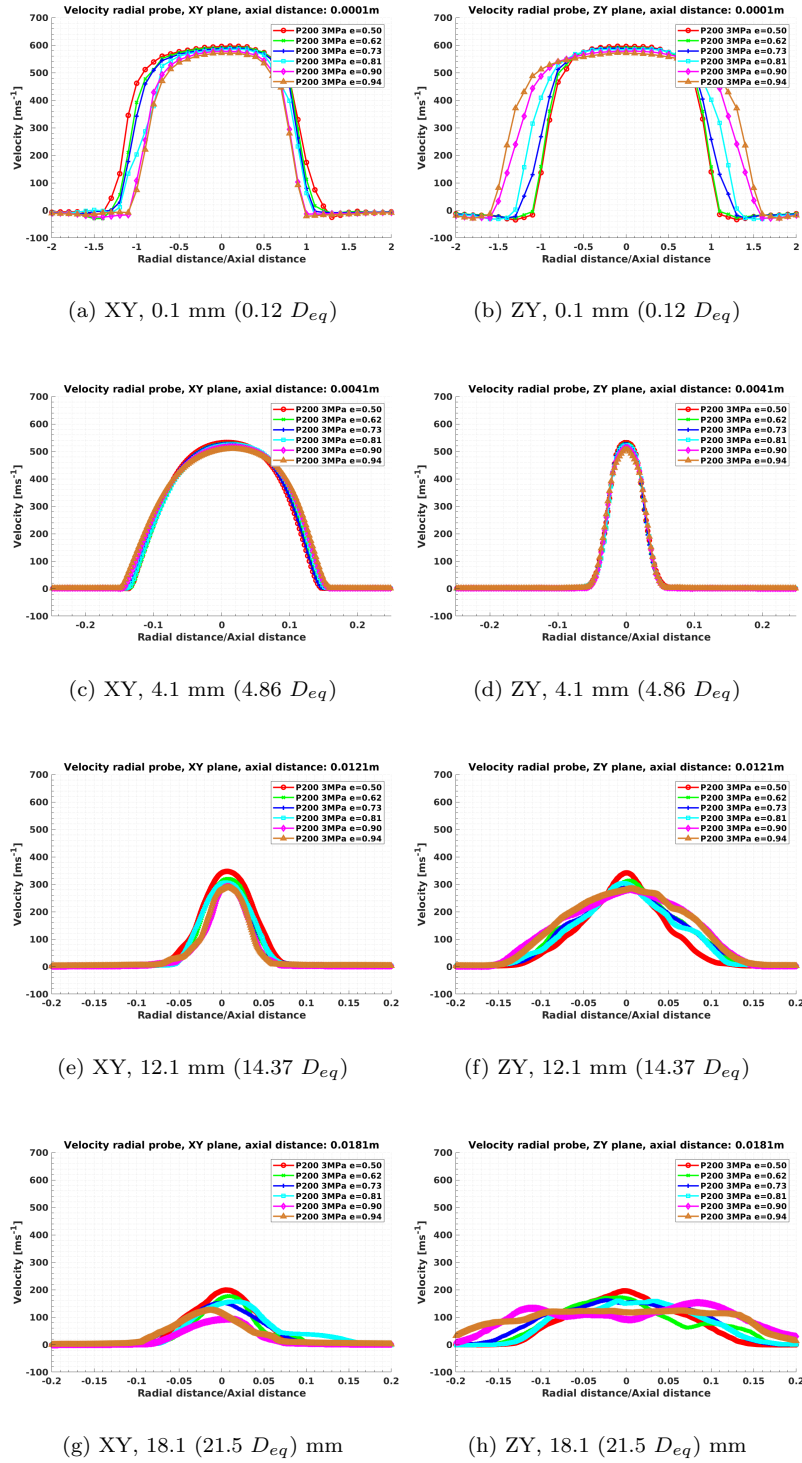


Figure 16: Radial velocity profiles for the elliptical nozzles.

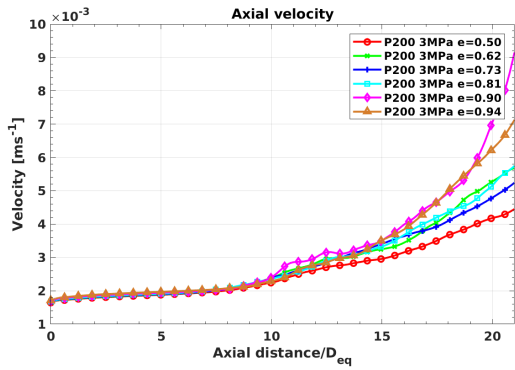


Figure 17: Axial liquid velocity

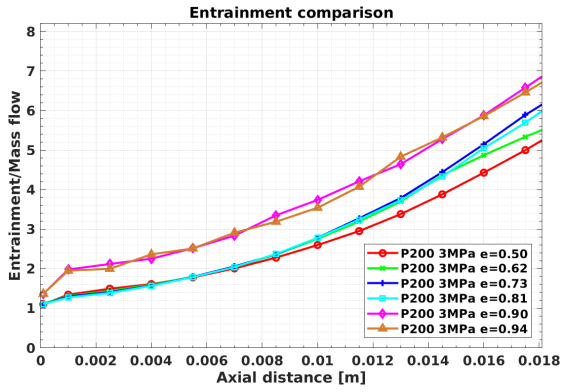


Figure 18: Jet entrainment.

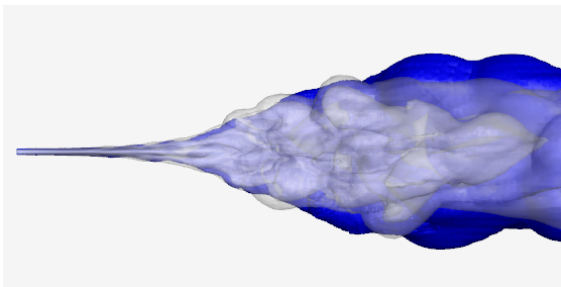


Figure 19: Iso-volume for a liquid mass fraction value of 0.01, ZY visualization plane. The nozzle of 0.50 eccentricity is depicted in white, the nozzle of 0.94 in blue.

860 that of the diesel nozzle of the present paper (Figure 861 13). As exposed by Ku et al. (2011), this fact produces a greater spreading angle in the major axis 862 (ZY plane). 863

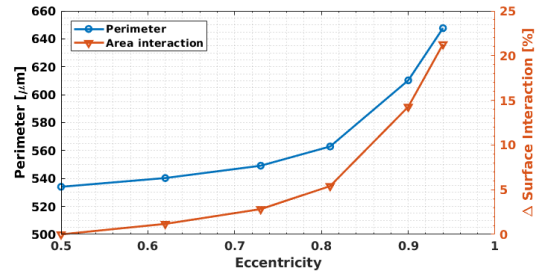
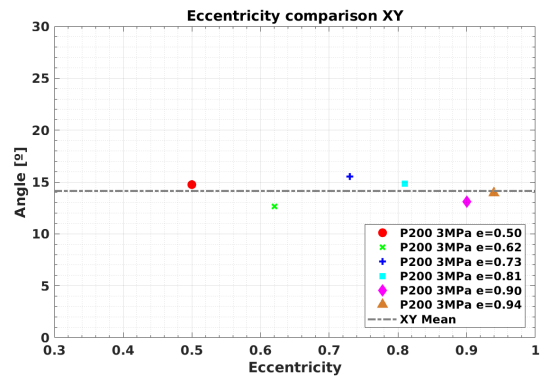
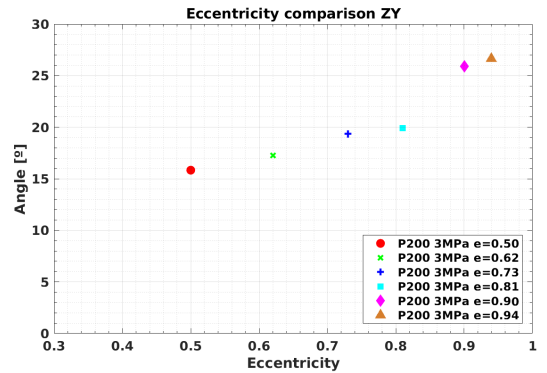


Figure 20: Geometrical effects of eccentricity over the spray interaction.



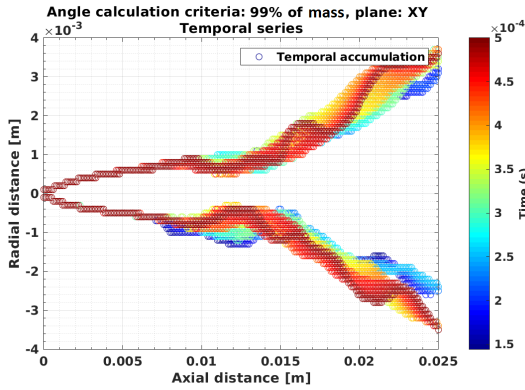
(a) Mean angle comparison in the minor axis plane (XY).



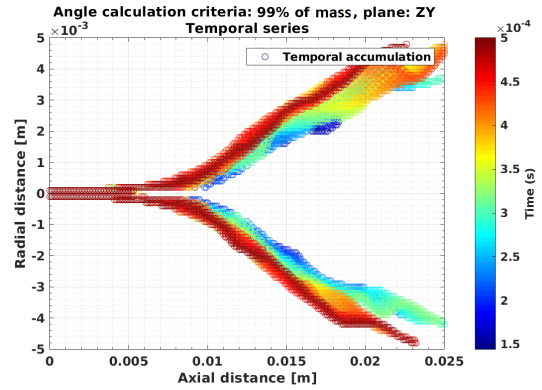
(b) Mean angle comparison in the major axis plane (ZY).

Figure 21: Angle comparison, elliptical nozzles.

864 Figure 22a depicts the temporal evolution of the 865 angle for the nozzle simulation with highest aspect 866 ratio ($e = 0.94$). A first view on the right side of 867 Figure 5 shows an almost constant angle for the 868 first millimetres of the spray up to 8 mm. At this 869 point, the angle starts to grow and the trend is 870 more significant. It is coherent with the absence of 871 higher disturbances at the nozzle outlet on the ex-



(a) Plane XY, minor axis



(b) Plane ZY, major axis

Figure 22: Temporal variation of angle, eccentricity = 0.94.

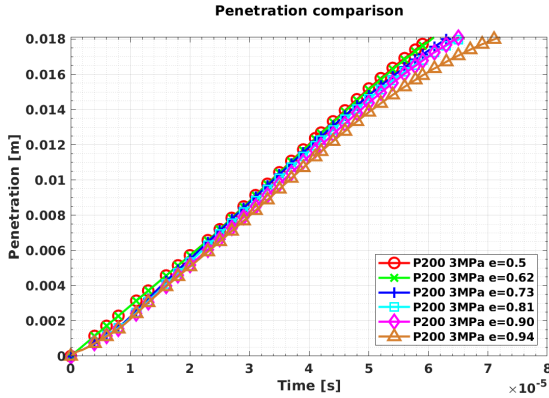


Figure 23: Penetration curves for the elliptical nozzles at full needle lift.

872 tremes of the major axis, unlike Kun et al. Image
 873 22a traces a complete different behaviour from the
 874 computational angle. The minor axis plane (XY)
 875 angle strongly grows first millimetres of the spray.
 876 This issue is explained by the high disturbances at
 877 the outlet in the XY plane according to the existence
 878 of cavitation. Beyond 8 mm the XY angle
 879 suddenly reduces its growth. It can be seen how
 880 both XY and ZY angles share the inflexion point
 881 at which its width trends switch. As previously
 882 commented, the XY plane is expected to have a
 883 wider angle. For cylindrical nozzles, the spreading
 884 of fuel is enforced by cavitation generating a almost
 885 axi-symmetric and wider spray that non cavitating
 886 cylindrical nozzles. In related studies (Ho and Gut-
 887 mark, 1987; Husain and Hussain, 1991; Hussain and
 888 Husain, 1989; Krothapalli et al., 1981), a switching

889 axes behaviour has been repeatedly detected. In
 890 these works, the anomaly in the spray behaviour
 891 compared to cylindrical nozzles was attributed to
 892 a self-induced vortex of the elliptical spray. One
 893 similar behaviour was described by Yu et al. (2018)
 894 in experiments with single-hole nozzles. Although
 895 the bibliography above has only exposed single-hole
 896 nozzles, and it can not be directly compare to those
 897 of this study, several of its physical phenomena can
 898 be extrapolated to the performance of multi-hole
 899 nozzles. Figure 24 depicts the switching axis be-
 900 haviour, first frames 24a, 24b, 24c and 24c shows
 901 the initial greater opening of the angle in the minor
 902 axis due to the effect of cavitation, the minor axis
 903 becomes the major axis. From frames 24d to 24i
 904 the instabilities start to rise in the new minor axis
 905 and it breaks in an inflexion point. The switching
 906 axis occurs between 24j and 24l. In picture 24m
 907 to 24t the greater dispersion in the ZY plane (geo-
 908 metrical major axis) starts to form a new and more
 909 defined elliptical shape. Summarizing, the general
 910 angle grows as the eccentricity rises being this fact
 911 more noticeable in the ZY angle (major axis) while
 912 in the minor XY axis the angle is at least as much
 913 bigger as the more cylindrical one.

A final outline over the problem commands the
 exam of penetration. Even if the simulations have
 been accomplished with a full needle lift, differences
 supporting the earlier discussion can be observed.
 Figure 23 provides the temporal evolution of pene-
 tration for all cases. As expected, a wider angle
 (high eccentricity values) generates a slower pene-
 tration curve (Desantes et al., 2006; Gimeno et al.,
 2016). However, it is true that in terms of pene-

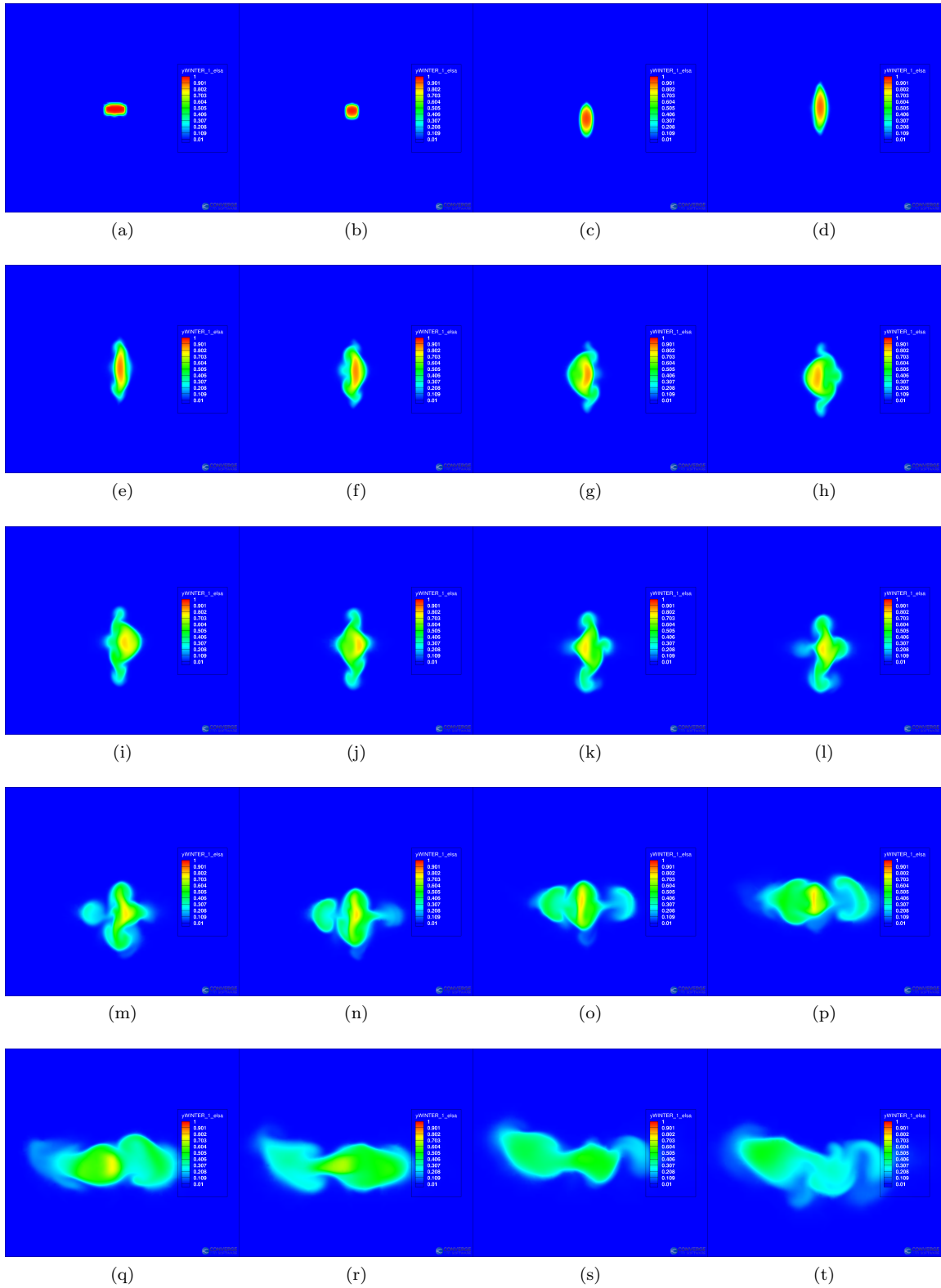


Figure 24: Main injection axis rotation due to self-induced vorticity of the jet, CFD.

923 tration, the difference between the nozzle 4 and 6 972
 924 is not as big as it could be suggested by previous 973
 925 data. The evolution of the jet further from this 974
 926 point is an interesting topic, specially for big en- 975
 927 gines. Unfortunately, computational resources have 976
 928 limited the simulation space and the injection du- 977
 929 ration. For future works, larger time injections in 978
 930 order to clarify both angles behaviours must be car- 979
 931 ried out for a better understanding of this kind of 980
 932 nozzles. Even so, it has been demonstrated that the 981
 933 general influence of eccentricity enforces the spray 982
 934 atomization by means of a wider angle. Also, it has 983
 935 been discussed how the internal parameters such as 984
 936 momentum and mass flow, are not enough for fully 985
 937 describing the spray atomization potential and how 986
 938 the entrainment and fluid fraction along the spray 987
 939 are in resonance with the angle and entrainment. 988
 940 The increment of the surface area of jet-air interac- 989
 941 tion and the momentum thickness must be consid- 990
 942 ered along with the self behaviour of the generated 991
 943 spray for the correct understanding of elliptical jets. 992
 944 A more complex model such as LES or near field 993
 945 DNS simulations could provide more specific data 994
 946 to measure these parameters. 995

947 6. Conclusions 996

948 Several elliptical nozzles with the same outlet 997
 949 area and different eccentricity have been simulated 998
 950 coupling the inner nozzle flow and spray formation 999
 951 by means of an advanced CFD code. The code has 1000
 952 been previously validated in terms of the nozzle hy- 1001
 953 draulic performance and spray formation for both 1002
 954 a single-hole conical nozzle as well as a multi-hole 1003
 955 cylindrical one. In the case of the latest, the sim- 1004
 956 ulation included the activation of a HRM model, 1005
 957 which accurately predicted the mass flow collapse 1006
 958 induced by cavitation. This multi-hole geometry 1007
 959 has been taking as a reference to produce the ellip- 1008
 960 tical geometries. 1009

961 The main conclusions of the study are summa- 1010
 962 rized below: 1011

- 963 1. A new study showing in depth the capabilities 1012
 964 of elliptical nozzles in order to improve the at- 1013
 965 omization and mixing processes has been car- 1014
 966 ried out by means of a numerical CFD model 1015
 967 coupling the internal nozzle morphology and 1016
 968 the external spray performance. 1017
- 969 2. The $\Sigma - Y$ model is able to capture the in- 1018
 970 ternal geometric morphology of the nozzle and 1019
 971 translate its characteristics to the spray. 1020

3. For an equal area and boundary conditions, in- 1021
 creasing the eccentricity for horizontal ellipti- 1022
 cal nozzles improves the discharge and area co- 1023
 efficients due to lower cavitation. The velocity 1024
 coefficient is slightly decreased, producing very 1025
 similar outlet momentum. In terms of cavi- 1026
 tation, such geometries induce a vapour field 1027
 with lower intensity but more dispersed across 1028
 the outlet section of the orifice. 1029
4. The spray behaviour has shown to be sensitive 1030
 to the nozzle flow characteristics. In this sense, 1031
 the spray cannot be fully understood only by 1032
 simple average parameters at the nozzle outlet, 1033
 which are the ones normally achievable with 1034
 experimental tools. The way the nozzle shape 1035
 interacts with the discharge chamber is critical. 1036
5. In terms of spray characteristics, more ellipti- 1037
 cal nozzles produce an improvement of air en- 1038
 trainment, with the minor angle showing small 1039
 variations, while the major angle increases sig- 1040
 nificantly. Consequently, spray penetration 1041
 tends to be reduced. 1042
6. A significant increment of the angle and jet 1043
 entrainment as the eccentricity rises are an in- 1044
 dication that elliptical nozzles can help to im- 1045
 prove the spray atomization processes. 1046

Some of the aforementioned features found have been also confronted with previous literature works, providing consistent trends.

1047 Declaration of conflicting interests

The author(s) declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

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