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Investigation of cavitation and air entrainment during pilot injection in real-size multi-hole diesel nozzles

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Abstract

This paper investigates the complex multiphase flow developing inside the micro-orifices of diesel injector nozzles during pilot injection. High speed micro-visualisations of a transparent serial production nozzle tip replica are used to record the multiphase flow inside the flow orifices as well as near-nozzle spray development. The physical processes taking place are explained with the aid of a three-phase (liquid, vapour and air) homogeneous mixture model utilized in the context of Large Eddy Simulations. Phase-change due to cavitation is considered with a model based on the Rayleigh-Plesset equation, while compressibility of all the phases is accounted for. Numerical simulations shed light on the interaction between the vortex flow and cavitation formation that take place simultaneously with air entrainment from the surrounding environment into the injector's sac volume during the injec-

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tion and the dwell time between successive injections. The experimentally observed flow phenomena are well captured by the simulation model. In particular the compression of pre-existing air bubbles inside the injector's sac volume during the injector opening, cavitation vapor condensation and air suction after the needle closure are well reproduced.

Keywords: LES, Multiphase flow, Cavitation, Fuel Injection, Pilot injection, Air entrainment

1. Introduction

New European Real Driving Emission (RDE) driving cycle legislations require significant research efforts to develop emission compliant and efficient passenger car engines [1]. In this context, the so-called digital injection schemes, used to split the fuel injection into multiple small injections with close separation among them, are widely applied in modern diesel engines in order to obtain simultaneous reductions in noise and emissions without compromising engine performance and fuel consumption [2, 3]. Although the nozzle flow for static needle lift conditions has been extensively investigated (see selectively [4, 5, 6, 7]), not much work is available for the flow development during the dynamic operation of the injector, which plays a key influence on emissions [8, 9].

The digital injection schemes are often operated with fast injector needle opening and closing and with very small separation between injections; with typical dwell time of the order of $50\mu s$. This results in highly transient flow

Nomenclature

α_{air}	air volume fraction	[-]	D	injection hole diameter	[m]
α_{liq}	liquid fuel volume fraction	[-]	E	total energy	[J/kg]
α_{nuc}	nuclei content	[-]	F_{vap}, F_{cond}	empirical constants	[m^{-1}]
α_{vap}	vapor fuel volume fraction	[-]	p	pressure field	[Pa]
\mathbf{v}	velocity field	[m/s]	R	gas constant	[J/kg/K]
λ_g	Taylor length scale	[m]	R_b	bubble radius	[m]
μ	viscosity	[Pa s]	R_e, R_c	evaporation/condensation rate	[$kg/m^3/s$]
μ_t	turbulent viscosity	[Pa s]	Re	Reynolds number	[-]
ρ	density	[kg/m^3]	T	temperature	[K]
ρ_{vap}, ρ_{air}	vapour/air density	[kg/m^3]	y^+	non-dimensional wall distance	[-]
σ	viscous stress tensor	[Pa]			
τ_t	turbulent stresses	[Pa]			

16 and formation of cavitation inside the injection nozzle. In addition, modern
 17 diesel engines are operated under high injection pressure ($> 2500bar$) and
 18 utilise injectors with small injection hole diameters ($90 - 120\mu m$); these con-
 19 ditions pose significant difficulties in measuring and/or optically visualising
 20 the processes occurring in both the injector nozzle and within the high tem-
 21 perature combustion chamber. The majority of transparent real-size nozzle
 22 investigations featuring simplified single-hole geometries that generally con-
 23 firm the presence of geometric-induced cavitation [10, 11, 12]. The work
 24 of [13, 14, 15], and the relevant early modelling work [16] were the first to

25 substitute one of the holes of a production nozzle with a quartz window of
26 identical geometric characteristics and was an experimental breakthrough
27 that provided valuable information on flow and cavitation structures inside
28 such micro-channels under realistic operating conditions; further studies were
29 reported in [17]. A step forward was realised in [18], where a 3-hole, real-
30 size, fully transparent nozzle allowed for unobstructed optical access inside
31 the sac volume. Vortex cavitation is dramatically enhanced by vapour or air
32 already present inside the nozzle volume [19]. Moreover, [20] showed that
33 the structure of a vortex core is significantly affected by entrained vapour
34 bubbles. Similarly, [21] demonstrated possible fragmentation of the vortex
35 core so as to increase the vorticity at the core centre. Finally, the strong in-
36 teraction observed between vortex properties and bubble dynamics[22], the
37 coupling of radial and axial growth of bubbles trapped in vortices [23] and
38 the interaction between shear (or normal strain) flow and bubble volume
39 change [24] form a tremendously complex flow field inside an injector noz-
40 zle, where dynamic changes in the behaviour of vortices and vapour bubbles
41 strongly affect the emerging fuel spray. Highly transient flow phenomena
42 caused by the fast needle response times, give rise to formation of vortical
43 structures and therefore, to string cavitation [25]. Transient effects have also
44 been correlated to increased probability of surface erosion damage, which
45 is attributed to both, geometric and string cavitation [26]. Cavitation in
46 simplified nozzle replicas has been visualized even at pressures as high as
47 2000bar, as shown in [27, 28]. Remarkably, in very recent studies, sonolu-

48 minescence from cavitation collapse observed in a simplified nozzle replica
49 has been observed for the first time[29] and a neutron imaging technique has
50 been developed overcoming the disadvantages of using materials transparent
51 to visible light[30]. All aforementioned studies report data from one or just
52 a few injection events. The group of the authors has reported in [31, 32, 33]
53 for the first time averaged images of cavitation developing in a real-size 6-
54 hole transparent tip nozzle for single and pilot-main split injections up to
55 400bar. Data from these investigations are further reported here and utilized
56 for validation of the newly developed model. Only the very recent work of
57 [34] has extended the range of operating conditions (injection pressures up
58 to 1000bar and back pressures up to 30bar) and geometrical features stud-
59 ied (hydro erosively ground inlet orifice) for long injections. These studies
60 provide qualitative data on cavitation and air-entrainment inside the fuel
61 injector during the opening and closing of the injector's needle valve. A
62 drawback of the images is that one cannot distinguish between cavitation
63 and air, as they both appear as an indistinguishable black shadow in the
64 obtained images.

65 Given the limited quantitative information around the flow structure in-
66 side diesel injectors, fuel injection equipment manufacturers require robust
67 predictive Computational Fluid Dynamics (CFD) tools, in order to under-
68 stand the physical mechanisms taking place during injection. From a physical
69 viewpoint, modelling of such flow conditions requires the fluid compressibil-
70 ity [35], mass transfer (cavitation, flash boiling, evaporation etc.) and heat

71 transfer [36, 37, 38] to be taken into account, which increase the complexity
72 as well as the computational cost of the simulations. Additionally, the fluid
73 dynamics processes occur at high Reynolds number and therefore accounting
74 for the effect of turbulence structures and vortex dynamics, is key in explain-
75 ing how the injected fuel spray is formed [39, 40, 41, 42]; this can only be
76 resolved using very fine computational grids and scale resolving simulations,
77 such as Large Eddy Simulation (LES).

78 Recent LES including dynamic needle movement for the in-nozzle flow
79 includes the work of Battistoni et al. [43] who simulated the start and end
80 of injection for a single hole nozzle using the cut cell cartesian method for
81 modelling the boundary movement and a homogeneous relaxation model for
82 cavitation phenomena. The work concludes that URANS predictions for the
83 residual liquid back flow occur without fragmentation, while in LES liquid
84 breaks up generating complex three dimensional structures. The URANS ap-
85 proach predicted at the end of the injection an annular void region stemming
86 from the needle seat, which then re-condenses as the pressure is recovered.
87 This was not observed in LES, where regions of low pressure are produced
88 even in areas detached from the needle seat. The predicted near spray region
89 was also different as no ligaments were formed in URANS; instead diffusion
90 disperses the liquid in the surrounding air even if integral values like sac
91 pressure and liquid volume fraction were not greatly affected. Ligament for-
92 mation and gas ingestion into the nozzle at the end of injection are predicted,
93 as observed experimentally in Phase Contrast X-ray images (for additional

94 Phase Contrast X-ray studies see for example [9, 44]). The start-of-injection
95 simulation shows how gas is ejected first, and liquid fuel starts being injected
96 with a delay. The main result of these analyses is that if the sac volume is
97 initially filled with gas, the liquid exit is delayed several tens of μs after the
98 start of needle movement, which is in good agreement with the experimen-
99 tal evidence. This delay is of the order of $100\mu s$, and it is compatible with
100 the duration of the first slow rising part of the needle movement. Orley et
101 al. [45] used the cut cell cartesian method to simulate with implicit LES, a
102 barotropic homogeneous equilibrium model for cavitation and a fully com-
103 pressible 3-phase flow model a complete 9-hole diesel injector. The focus of
104 the work was on the vortical development of the flow and the assessment
105 of erosion sensitive areas during the operation of the injector. After the in-
106 jector closing, strong collapse events of vapor structures in the needle seat
107 and the sac hole cause the formation of violent shock waves. The authors
108 highlighted that a fully compressible description of the flow is essential to
109 capture such phenomena. It was also concluded that despite steady needle
110 simulations capturing the main flow features reasonably well, vapor creation
111 during the closing phase of the needle valve requires information on the pre-
112 viously developed flow; thus, reliable prediction of erosion-sensitive areas
113 due to collapse events during and after the closing of the needle can only
114 be predicted accurately by including the unsteady needle motion. Finally,
115 the work of Koukouvinis et al. [35] used a 2-phase dynamic needle approach
116 based on a combination of layering and stretching algorithms together with

117 a Rayleigh-Plesset based cavitation model with increased mass transfer, to
118 compute the opening phase of two different injector designs; the findings
119 have correlated the pressure peaks in the domain with areas that suffer from
120 erosion. Whichever the chosen modelling approach may have been, previous
121 studies have lacked validation [45], had indirect validation [35] or were not of
122 direct relevance to modern applications [43], since a single hole nozzle lacks
123 the complex sac recirculation flow present in modern diesel injectors.

124 On the broader perspective, reduction of exhaust gas and in the same
125 time noise emissions from engines, relies on multiple injection strategies,
126 such as digital rate shaping (DRS) [46, 47, 48, 49], which allow the use of a
127 variety of options for pilot, main, and post-(main) injection events in order
128 to provide a degree of control over the timing and phasing of the ignition
129 delay and heat release events, as reported in [50]. Recent investigations from
130 the group of the authors suggest that when the dwell-period is shortened,
131 there is significant reduction in soot while exhaust-out NO_x is controlled by
132 EGR. Similarly, the CN-soot trade-off can be decoupled by reducing pilot-
133 main dwell time, adding a greater number of pilots and increasing rail pres-
134 sure without compromising fuel consumption [51]. The use of such complex
135 strategies described relies on the ability of the fuel injection equipment to
136 accurately meter extremely small quantities of fuel per event (which may be
137 of the order of $1mg$ of fuel being injected in a period of less than $0.25ms$)
138 over the engine lifetime [49]. During these short metering events the injector
139 will not reach full lift and will be operating within the transient part of the

140 rate curve. To meet these demands, it is extremely important to avoid the
141 accumulation of excessive carbonaceous deposits on, and within the fuel in-
142 jector. Nozzle hole deposits can reduce the effective flow area of the fuel or
143 cause it to be mis-directed. These effects give rise to poorer atomisation and
144 mixing, excessive spray penetration, and increased risk of fuel impacting on
145 the combustion chamber surfaces, with the potential to adversely affect emis-
146 sions. The impact of deposit formation within nozzle holes and their effect
147 on engine performance are well summarised in [52], concluding that residual
148 fuel remaining within the injector nozzle's sac and holes are thought to be
149 instrumental in the process [9]. With increasing number of pilot injections
150 with short dwell time, the residual fuel in the nozzle sac after needle closure
151 can be critical for the HC and soot emissions. However, experimentation of
152 the detailed flow dynamics inside the injector at such conditions is practi-
153 cally impossible; currently there is no study reporting quantitative data on
154 the flow development during the injection events for such processes. The
155 experimental data reported in [31, 32, 33, 34] clearly indicate that the flow
156 and cavitation development inside the injector is different in every injection
157 cycle, and differ significantly from the experimentally derived time-averaged
158 field, as shown in [32]. An alternative to shed light to those processes, is the
159 use of computational fluid dynamics. The current work, to the best of the
160 authors knowledge, presents for the first time application of a 3-phase LES
161 to the flow in a diesel injector for a pilot injection event, including cavitation
162 and compressibility of all phases; simulations have utilised the optically mea-

163 sured needle valve movement from fully transparent real size 6-hole nozzle
164 tips [31, 32, 33], as reported by the group of the authors. Moreover, the
165 high-speed shadowgraph images from those studies serve as validation of the
166 developed model; these include the location/timing of cavitation initiation,
167 its further extent and eventual collapse and the air entering into the injection
168 holes and sac volume of the nozzle tip.

169 The need to employ LES derives from the necessity to predict the flow
170 formation of individual injection cycles, as opposed to cycle-averaged flow
171 distribution. The complexity of the flow is not only linked to the formation
172 of cavitation, but also to the residual air present inside the injector; this has
173 been considered in the present work by initialising the residual air distri-
174 bution inside the injector’s sac volume and injection holes from the images
175 recorded for individual injection events. Moreover, inclusion of compress-
176 ibility effects for all phases is deemed as necessary for resolving the complex
177 liquid, cavitation formation and development and air compression/expansion
178 inside the injector, as it is shown in the reported results.

179 The present paper is structured in the following way: first an overview
180 on the experimental results is given for a diesel pilot injection visualization
181 of a transparent nozzle tip. Then the numerical methodology employed is
182 described in detail, followed by the comparison of the CFD results with the
183 transparent nozzle visualisations for which good agreement is obtained and
184 interpretation of the observed phenomena is provided.

185 2. Experimentally observed multiphase phenomena

186 As already mentioned, the 3-phase simulation methodology has been val-
187 idated against high speed visualisations of a transparent Delphi Technologies
188 Diesel 6-hole nozzle tip manufactured by City, University of London. The
189 metallic injector nozzle tip was substituted with a transparent acrylic tip.
190 The design is a standard serial production geometry, i.e not just a multi-hole
191 nozzle, but a fully operational, serial production type. The detailed results
192 and findings of that experimental campaign as well as the setup details were
193 reported in [31, 32, 33] and will not be repeated here. The 6-hole transparent
194 tip has holes with no taper (zero conicity) and a nominal diameter (D) of
195 $160\mu m$. The electrical pulse activation width for a pilot injection was $0.5ms$.
196 High speed cameras recorded the events at a frame rate of $30000fps$. An
197 example of a pilot injection for a rail pressure of 300bar into atmospheric
198 conditions can be found in Figure 1. Given the image acquisition rate, the
199 pilot injection including all major events after closing lasts for 24 frames.
200 As discussed in [32, 33] air trapped in the sac after the end of the injection
201 aggregates forming bubbles in the sac and occupying part of the hole. Prior
202 to $233.33\mu s$ after the electrical trigger, no change is observed and therefore
203 images are not shown. Then the trapped bubble shows slight expansion due
204 to the initial volume created by the needle as it starts lifting ($300\mu s$ after
205 the trigger) and subsequent compression ($400\mu s$ after the trigger) highlight-
206 ing the need to model air compressibility. This is followed by void coming
207 from the seat passage and its advection into the hole ($500\mu s$ after the trigger).

208 Then, due to flow acceleration at the hole entrance, void structures are seen in
209 the hole during the opening phase ($600\mu s$ after the trigger). During the nee-
210 dle closing phase, vapour increases substantially in the hole and void coming
211 from the seat reappears ($633.33\mu s$ after trigger). At the end of the injection,
212 the sac gets full with bubbles and the spray greatly weakens ($733.33\mu s$ after
213 the trigger), followed by what seems to be air suction ($766.66\mu s$ after the
214 trigger). Finally, a bubbly mixture is observed floating in the sac as well as
215 an oscillatory movement of the air in the hole ($1000\mu s$ after the trigger). An
216 important input for nozzle flow moving needle simulations is the needle lift
217 profile which was extracted from the images [31, 32, 33].

218 **3. Modelling approach**

219 The simulations are computed using the commercial CFD code ANSYS
220 Fluent [53]. The nozzle flow is solved using a homogeneous, three-phase
221 mixture model (liquid fuel, vapour fuel and air) where all phases share the
222 same velocity, pressure and temperature. The code is supplemented with
223 user defined functions (UDFs) for implementation of the thermo-hydraulic
224 properties of diesel and the needle movement.

225 *3.1. Multiphase model*

226 The properties appearing in the transport equations are determined by
227 the presence of the component phases in each control volume. Defining α_{liq} ,
228 α_{vap} , α_{air} as the volume fraction of liquid fuel, air and vapour fuel in a cell,



Figure 1: Experimental results. Time sequence of a pilot injection transparent nozzle tip visualisation.

229 respectively, the density in each cell is given by: $\rho = \alpha_{liq}\rho_{liq} + \alpha_{vap}\rho_{vap} +$
 230 $\alpha_{air}\rho_{air}$.

231 All other transport properties (viscosity and thermal conductivity) are
 232 computed in this manner despite the fact that for homogeneous mixtures it
 233 is not clear how one should average each phase's effect, whether based on
 234 mass, volume or area (which would require knowledge of interfacial surface-
 235 area density). Although in the case of bubbly flows some theoretical deriva-
 236 tions attributed to Einstein do exist [54], viscosity in general depends non
 237 linearly on the void fraction and in order to achieve accurate pressure drop
 238 calculations the mixture viscosity has to be empirically corrected by fitting
 239 coefficients to match experimental data sets [55]. For a review on the avail-
 240 able correlations for the transport properties the interested reader is referred
 241 to [56]. Obviously, the volume constraint $\alpha_{liq} + \alpha_{air} + \alpha_{vap} = 1$, in each cell
 242 must be respected. The solved equations consist of the continuity, momen-
 243 tum and energy of the mixture, and the mass conservation equations for the
 244 vapor and the air:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \quad (1)$$

$$\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = -\nabla p + \nabla \cdot \sigma \quad (2)$$

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot (\mathbf{v}(\rho E + p)) = \nabla \cdot (k_{eff} \nabla T) + \sigma \cdot \mathbf{v} \quad (3)$$

$$\frac{\partial \alpha_{vap} \rho_{vap}}{\partial t} + \nabla \cdot (\alpha_{vap} \rho_{vap} \mathbf{v}) = R_e - R_c \quad (4)$$

$$\frac{\partial \alpha_{air} \rho_{air}}{\partial t} + \nabla \cdot (\alpha_{air} \rho_{air} \mathbf{v}) = 0 \quad (5)$$

245 The source terms R_e and R_c represent the mass transfer between liquid
 246 and vapour phase due to cavitation. The effective viscous stress tensor is
 247 defined as $\sigma = \tau + \tau_t = \mu(\nabla v + (\nabla v)^T) + \tau_t$,

248 where μ is the viscosity of the mixture and τ_t are the turbulent stresses
 249 defined per the turbulence model being used. The energy is computed as the
 250 mass average for each phase and the internal energy of each phase is based
 251 on the local thermodynamic conditions of that phase [37].

252 The source terms appearing in the vapour volume fraction transport equa-
 253 tion ($R_e - R_c$) represent the mass transfer between fuel liquid and vapour
 254 phases due to cavitation bubble expansion and collapse respectively. The
 255 calculation of these values is based on the Rayleigh-Plesset equation describ-
 256 ing bubble expansion and collapse [57], and its magnitude is based on the
 257 Zwart-Gerber-Belamri cavitation model [58] which reads as:

$$R_e = F_{vap} \frac{(3\alpha_{nuc}(1 - \alpha_{vap})\rho_{vap})}{R_b} \sqrt{\frac{2 \max((p_{vap} - p), 0)}{3 \rho_{liq}}} \quad (6)$$

$$R_c = F_{cond} \frac{(3\alpha_{vap}\rho_{vap})}{R_b} \sqrt{\frac{2 \max((p - p_{vap}), 0)}{3 \rho_{liq}}} \quad (7)$$

258 F_{vap} and F_{cond} are empirical calibration coefficients, α_{nuc} is the volume
 259 fraction associated with the nuclei contained in the liquid and R_b the assumed
 260 bubble radius and p_{vap} is the vapour pressure. According to [58], values of
 261 $R_b = 10^{-6}m$, $\alpha_{nuc} = 5 \times 10^{-4}$, $F_{vap} = 50$, $F_{cond} = 0.01$ give reasonable re-
 262 sults in a wide range of flows. Nevertheless, as discussed in [59] the mass
 263 transfer magnitude for these values could be insufficient creating areas of
 264 unrealistic liquid tension and not reproducing correctly the Rayleigh-Plesset
 265 bubble collapse, the suggested solution is to increase the empirical calibra-
 266 tion coefficients several orders of magnitude to approximate the model to
 267 a Homogeneous Equilibrium Model (HEM). However, within this work the
 268 original coefficients published in[58]were used.

269 3.2. Turbulence model

270 The target when using LES is to capture the large scales that are depen-
 271 dent of the physical domain simulated while modelling the sub-grid turbulent
 272 scales. This is achieved by filtering of the Navier-Stokes equations using a
 273 spatial low-pass filter determined by the cell size of the computational domain
 274 used. This operation leaves the flow equations unchanged, but transforms
 275 the equations into equations for the filtered magnitudes [60]. During this
 276 operation terms in the equations appear representing the sub grid scale con-
 277 tributions to the equations of motions and have to be modelled. The closure
 278 of the model requires calculating a suitable sub grid turbulent dissipation
 279 (viscosity) μ_t . For such purpose, the Wall-Adapting Local Eddy-Viscosity

280 (WALE) model is chosen [61]. This model is capable of correctly reproduc-
281 ing the correct turbulence wall behaviour ($\mu_t \sim o(y^3)$) and becomes 0 at
282 $y = 0$, being y the normal distance to the wall. Another advantage is that
283 it returns a zero turbulent viscosity for laminar shear flows which allows
284 the correct treatment of laminar zones in the domain, this is necessary for
285 modelling the start of injection when flow velocities are low.

286 3.3. Fluid properties

287 High injection pressures and low lifts cause high injection velocities and
288 transient heating effects making an incompressible approach unjustifiable
289 [36, 37, 35]. Even if for the transparent nozzle tip testing conditions the
290 pressure is lower than engine conditions, the diesel liquid phase is modelled
291 as a compressible liquid based on the measurements made for the calibration
292 oil Normafluid ISO4113. This is the usual fuel for testing and calibrating
293 diesel fuel injection systems in both laboratories and at an industrial level.
294 All diesel properties that follow are taken from [62, 63], where details of the
295 measurement methodology, range of validity, method for fitting the coeffi-
296 cients and their values can be found (see Figure 2 for plots of the density and
297 viscosity values for different pressures and temperatures). These properties
298 were implemented into ANSYS Fluent following the available User-Defined-
299 Real-Gas-Model (UDRGM) functionality as in [37]. As mentioned in the
300 experimental results section, air compressibility effects are observed during
301 the sac filling event and therefore the air density is modelled as an ideal gas

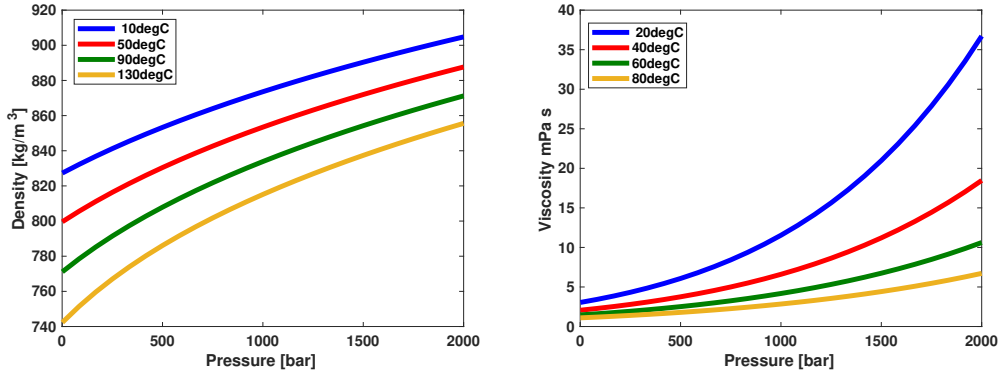


Figure 2: Diesel fuel properties implemented. Density (left) and viscosity (right) diesel fuel properties used.

302 with equation of state $p = \rho RT$.

303 3.4. Moving mesh methodology. Mesh generation and boundary conditions.

304 Modelling the dynamic movement of the needle is inherently difficult. At
 305 low lifts the cells in the seat are squeezed into very small gaps deteriorating
 306 their quality, which can have an impact on the robustness and accuracy of the
 307 simulation. Moreover, the contact between walls is not trivial to model since
 308 the continuity of the mesh is broken. Recent advances have been reported
 309 in [50] where the immersed boundary method has allowed simulations to
 310 be performed even at zero needle lift; however, this method has not been
 311 adopted here and as a compromise, the closed needle is modelled using the
 312 seat surface as a wall when the needle lift is below $1\mu m$.

313 The approach followed is based on an interpolation approach between two
 314 topologically identical meshes (key-grids) with the same number of cells and
 315 was already employed by the authors in [64]. The initial mesh has a $1\mu m$

316 lift and the high lift mesh is based on the maximum lift reached for the pilot
 317 injection $36\mu m$. Based on the node position of this two meshes any interme-
 318 diate lift is achieved by linear interpolation between the node position of the
 319 two key-grids. Another difficulty associated is the loss of resolution in the
 320 seat passage as the needle reaches high lifts, this requires interpolating the
 321 results into another pair of key-grids such as in [37]. For the pilot injection
 322 cases considered here, this was not needed due to the relatively low lift at-
 323 tained ($36\mu m$). Moreover, in order to save computational resources, just a
 324 60° sector is model (one hole) based on the nominal (target) geometry. Figure
 325 3 (left) shows the computational domain, consisting of different surfaces; the
 326 hole, housing, needle, seat inlet and side surfaces. Additionally, a 2mm long
 327 conical discharge volume is added in order to move away the outlet boundary
 328 condition from the areas of interest. The computational mesh used for the
 329 LES flow simulation is a fully hexahedral mesh.

330 The LES settings are adapted from the basis of the previous successful
 331 studies on diesel [39, 40, 41, 42] and gasoline [64, 65] direct injection and
 332 primary breakup simulations. In order to choose the appropriate filter/mesh
 333 size for the LES, the Taylor micro-scales (λ_g) have been estimated. This
 334 length scale is the intermediate length scale at which fluid viscosity signif-
 335 icantly affects the dynamics of turbulent eddies in the flow [66]. For the
 336 flow inside the transparent tip, the Reynolds number based on the nozzle
 337 hole diameter, outlet pressure and inlet temperature can be estimated to be
 338 $Re = \frac{(\rho V D)}{\mu} \sim 13000$. The Taylor micro-scales can then be approximated by

339 [60]: $\lambda_g = \sqrt{\frac{10D}{Re}} = 4.4\mu m$. However, in order to resolve the smallest eddies
 340 close to the wall, the non-dimensional wall distance based on the friction
 341 velocity has to be of the order of 1 ($y^+ \sim 1$) [60]. Therefore, additional
 342 refinement close to the walls is needed. An estimate of this value based on
 343 the turbulent boundary layer theory yields a cell wall distance of $\sim 0.2\mu m$
 344 . In order to reach a value of $\sim 5\mu m$ in the bulk flow without increasing
 345 excessively the number of cells, a cell growth ratio of 1.1 was applied in the
 346 wall. Under these constraints, a $\sim 5M$ element mesh was produced, with a
 347 volume change between neighbouring cells below 3, minimum cell angle of
 348 27° and $3D$ determinant (normalized triple product of the vectors starting
 349 from each cell node) above 0.6 for both key-grids. Special care was taken to
 350 refine the needle seat area in the stream-wise direction in order not to exceed
 351 for low lifts aspect ratios of 100 in the direction of the bulk flow. Figure 3
 352 (right) depicts the two meshes needed for the interpolation method, and a
 353 front view of the mesh showing the additional refinement in the seat area.
 354 A pressure boundary conditions was applied to the inlet of the domain. The
 355 pressure at the injector entrance in the high-pressure pipe was taken from
 356 the experimentally recorded values for every individual injection event. Dur-
 357 ing the opening phase, pressure decreases at the injector entrance due to the
 358 increasing flow through it. At the end of the injection an over pressure is
 359 observed due to the water hammer effect after needle closing. The pressure
 360 at the entrance of the injector was provided in [31]. A temperature of $300K$
 361 was chosen for the flow entering the domain and an air mass fraction value

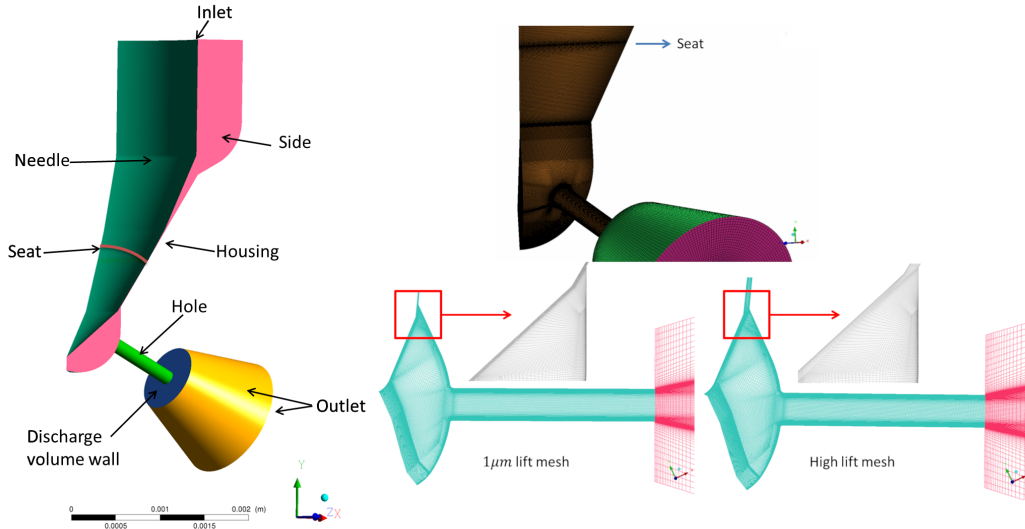


Figure 3: Geometrical model and mesh. Domain simulated and boundary conditions (left). Mesh showing seat refinement (right-top) and mesh cross section for both high and low lift meshes (right-bottom).

362 of 2×10^{-5} was imposed to take into account the possible dissolved air since
 363 it is a typical value for fuel or water exposed to ambient pressure [67]. The
 364 non-slip boundary conditions was applied to the non-moving wall (housing,
 365 hole, discharge volume wall, and, seat surface below $0.1\mu m$) as well as to
 366 the needle according to the motion profile resulting from the needle lift pro-
 367 file extracted from the images [31]. Periodic boundary condition have been
 368 applied to the side surfaces. Finally, a fixed pressure outlet was applied to
 369 the outlet surfaces, with pressure $1bar$ and $300K$ and air volume fraction
 370 prescribed as 1 in the case of back-flow.

371 The experimental images of the transparent nozzle show trapped air bub-
 372 bles inside the injector before the start of injection. The mechanism behind

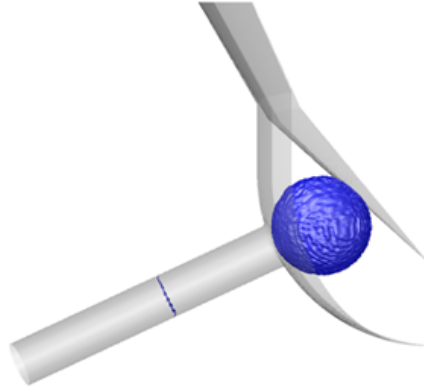


Figure 4: Initial simulation instant. Iso-surface of 0.5 liquid volume fraction and a mid-plane for the initial instant.

373 the appearance of this bubble is not straight forward to derive from the ex-
374 perimental images. Regardless, the LES nozzle flow simulation is initialised
375 in qualitatively similar way; half of the hole is filled with air and an air
376 spherical bubble is included in the sac (see Figure 4).

377 The computational domain above the seat surface is initialised at the
378 pressure corresponding to that instant. Below the needle seat, the simula-
379 tion is initialised at a pressure of $1bar$. All the domain is initialised at a
380 temperature of $300K$ and with zero velocity. For the closing phase the move-
381 ment of the needle is stopped when it reaches $1\mu m$ however the seat surface is
382 not switched from interior to wall until the needle lift profile reaches $0.1\mu m$.

383 The solver used is segregated and pressure-based. The pressure-velocity
384 coupling is achieved using the SIMPLEC algorithm [68]. Density is interpo-
385 lated using a second order upwind scheme [69] while for the momentum a
386 bounded central differencing scheme based on the normalized variable dia-

387 gram (NVD) approach together with the convection boundedness criterion
388 (CBC) [70] was used. The bounded central differencing scheme is a com-
389 posite NVD-scheme that consists of a pure central differencing, a blended
390 scheme of the central differencing and the second-order upwind scheme, and
391 the first-order upwind scheme. The first-order scheme is used only when the
392 CBC is violated. This scheme has small numerical dissipation and sufficient
393 numerical stability for industrial LES simulations [71]. Among the volume
394 fraction interpolation schemes available in ANSYS Fluent when using the
395 mixture model, the quadratic upstream interpolation for convective kinetics
396 (QUICK) scheme is selected in order to reduce the smearing of sharp volume
397 fraction gradients and capture high density ratios [72]. Pressure interpola-
398 tion follows the body force weighted scheme [53] and the temperature the
399 first order upwind scheme. Finally the calculation of gradients was done
400 using the Least Squares Cell-Based method.

401 The used solver is pressure-based and therefore the simulation stability
402 is not limited by the acoustic wave propagation time scale. However, tem-
403 poral resolution for LES requires minimum diffusion for the advection of the
404 turbulent eddies. Therefore, an adaptive time step method is employed to en-
405 sure the advection CFL number stays below 1 throughout the computational
406 domain.

407 *3.5. LES mesh quality evaluation*

408 The instantaneous fields of the LES quality metric of by Celik et al.[73]
 409 and y^+ for a representative moment at the highest lift ($t = 0.608ms$) are
 410 shown in Figure 5. Based on the y^+ the boundary layer resolution can be
 411 assessed; this value only exceeded 1 in areas above the seat and gradually
 412 transitions to values well under 1 ensuring a good wall shear resolution for
 413 the small eddies near the walls. Following [60] a good LES requires the
 414 modelled turbulent kinetic energy (k_{sgs}) to be less than 20 of the total tur-
 415 bulent energy ($k_{sgs} + k_{res}$), that is $\frac{k_{sgs}}{k_{sgs} + k_{res}} < 0.2$. However, as mentioned
 416 in [43] knowledge of k_{res} in the case of a moving needle injection can only
 417 be gained by repeating the simulation multiple times which could not be af-
 418 farded computationally. Although they are point indicative measures which
 419 are not particularly accurate for anisotropic turbulence, another option is to
 420 use metrics based on the turbulence resolution length scale such as the LSR
 421 metric; see for example [74] and its application by Battistoni et al. [43] to a
 422 moving needle injection, or the similar metric by Celik et al.[73]:

$$LESIQ_\nu = \frac{1}{1 + 0.05\left(\frac{\mu + \mu_t}{\mu}\right)^{0.53}} \quad (8)$$

423 where μ_t is the sub-grid scale viscosity introduced by the WALE model.
 424 This is a number between 0 and 1 for which the constants are calibrated such
 425 that the index is perceived similar to the ratio of resolved to total turbulent
 426 kinetic energy i.e. the higher the value the better the resolution is (0.8

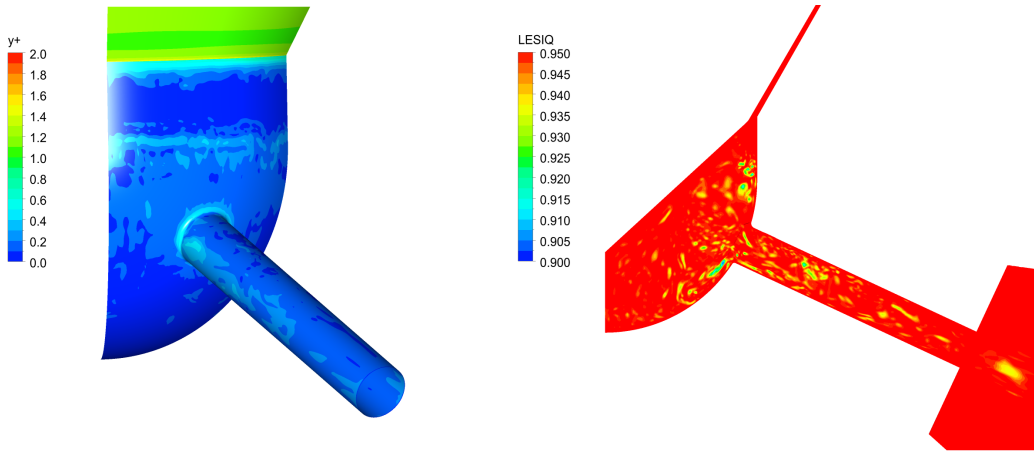


Figure 5: Mesh resolution evaluation. y^+ contours on the nozzle wall (left) and the LES quality metric of [73] (right) for highest needle lift during the pilot injection.

427 or above). Although [73] suggests to include as well the artificial viscosity
 428 introduced by the numerical methods, it is beyond the scope of this work to
 429 estimate such contribution. As seen in Figure 5 the value of $LESIQ_\nu$ for the
 430 same representative time instant is mostly over 0.95 throughout the domain
 431 and having a minimum values of 0.9 in the separation region that occurs at
 432 the entrance of the sac, confirming the suitability of the mesh.

433 4. Results and discussion

434 The evolution of the volume fraction inside the nozzle for the different
 435 phases is shown in Figure 6. Additionally, the imposed needle lift extracted
 436 from the image sequence shown in Figure 1 is shown as well. The simulation
 437 is started at the physical time $0.4874ms$ coincident with a lift of $1\mu m$ for
 438 the imposed profile. During the opening phase it follows from this plot that
 439 initially there is air present inside the nozzle. This air is evacuated out of

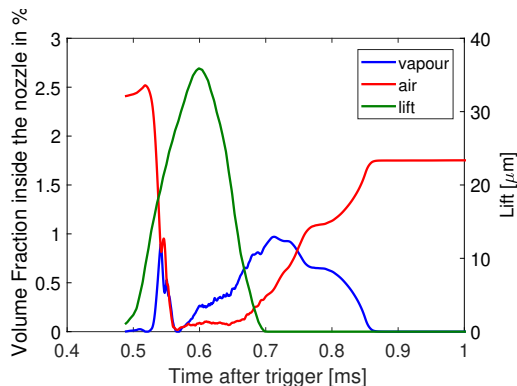


Figure 6: Integral results. Volume of vapour and air inside the nozzle and needle lift against time.

440 the nozzle while cavitation is generated showing a peak between $0.5ms$ and
 441 $0.6ms$, while it decreases afterwards. As the injection transitions towards
 442 the closing phase the amount of vapour increases, showing a peak just after
 443 the needle closes, while the amount of air continually increases by a process
 444 of air suction as it will be shown in the following section.

445 A comparison between the transparent nozzle tip images and the simula-
 446 tion results at the start of the injection is shown in Figure 7. In particular,
 447 a snapshot of the predicted liquid volume iso-surface of 50 at $t = 0.532ms$
 448 is shown. At the early stages of the injection the simulation reproduces the
 449 compression of the air bubble inside the sac volume. The compression is
 450 caused by the pressure build up in the sac, justifying the inclusion of the
 451 compressibility of the air. This is quickly followed by cavitation originating
 452 at the needle seat passage, due to flow separation and shear in this area.

453 Sample simulation results and the transparent nozzle tip images for the
 454 needle opening phase are shown in Figure 8. The CFD results indicate that

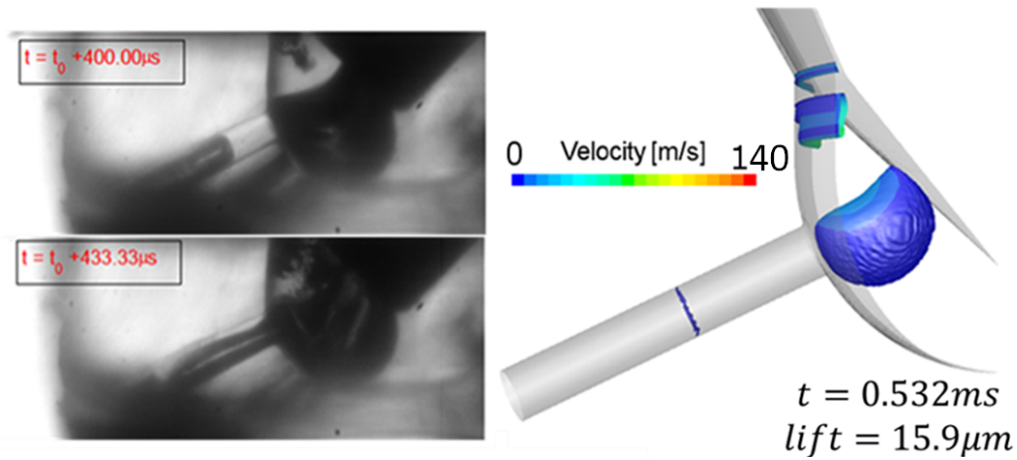


Figure 7: Start of injection results. Experimental visualisations (left), 50% liquid volume fraction iso-surface coloured by velocity magnitude (right).

455 cavitation produced at the sac entrance is transported directly into the in-
 456 jection hole. Simultaneously, the air bubble is further compressed and is
 457 pushed to recirculate parallel to the needle in the direction of the needle mo-
 458 tion. Similarly to the experimental images, the air bubble is seen breaking
 459 down and mixing with any remaining cavitation into a fine bubbly mixture
 460 which is then advected into the hole.

461 As the needle lift increases and the flow further develops, the simulation
 462 indicates that air disappears from the sac volume, as seen in Figure 9. This
 463 is attributed to a combination of two effects. Firstly, the sac pressure build
 464 up causes the air to be compressed, reducing its volume fraction. Secondly,
 465 as the air is trapped within the recirculation zone developing inside the sac
 466 volume, it enters into the injection hole, where it expands due to the local
 467 pressure drop at its entrance. This contributes to the void areas observed

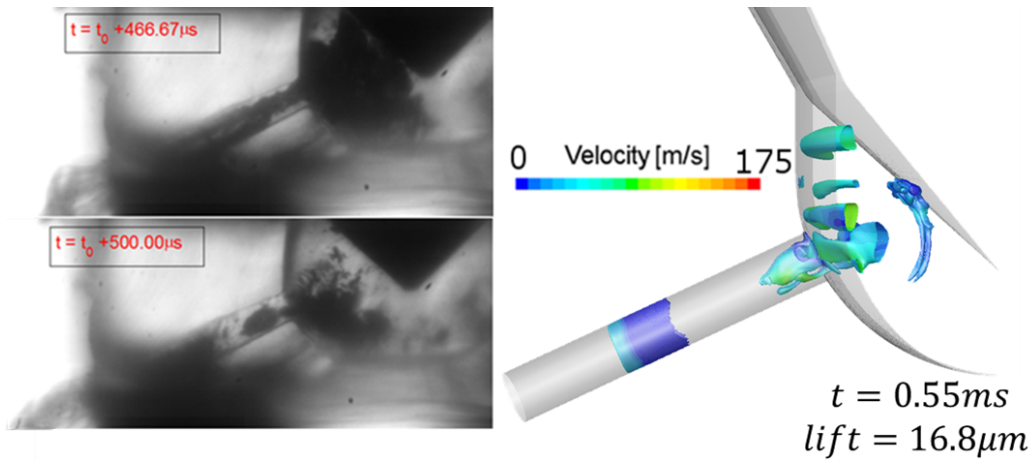


Figure 8: Needle opening phase results. Experimental visualisations (left), 50% liquid volume fraction iso-surface coloured by velocity magnitude (right).

468 and suggests that the void observed experimentally is a combination of air
 469 and fuel vapour. In addition, part of the void visible in the simulation can
 470 be attributed to geometrical cavitation developed at the hole inlet upper lip,
 471 which can be also seen from the experimental images.

472 The only two experimental frames available for the needle closing phase
 473 together with the simulation results are shown in Figure 10 (top). As the
 474 needle valve moves into the closing phase, the amount of void in the hole in-
 475 creases. This is in agreement with the simulation results from Figure 6, where
 476 volume content as a percentage of the injector volume of both air and vapour
 477 are plotted against time; it follows that these quantities increase during the
 478 needle closing phase. This void in the simulation has two sources, one from
 479 the unstable vortical flow developing inside the sac volume and entering into
 480 the injection hole and another due to formation of geometric-induced cavi-

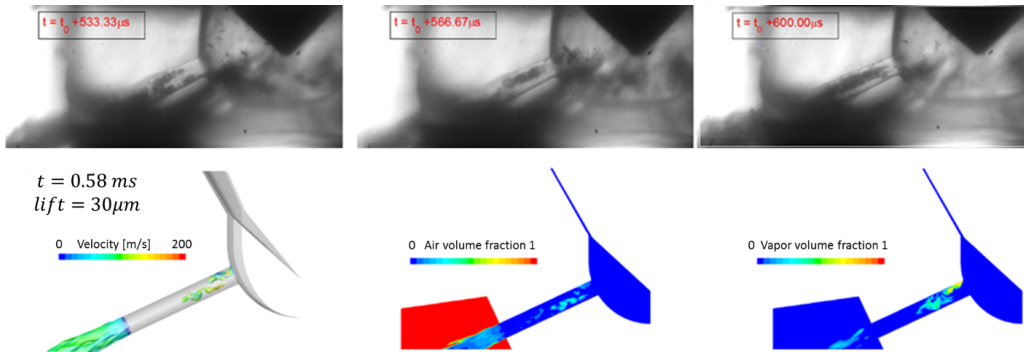


Figure 9: Results as flow further develops during the opening phase. Experimental visualisations for three time instances (top), 50% liquid volume fraction iso-surface coloured by velocity magnitude (bottom-left), air volume fraction contours (bottom-centre) and vapour volume fraction contours (bottom-right).

481 tation at the hole inlet corner. Regarding the experimental results at very
 482 low lifts ($lift = 6\mu m$), a bubbly mixture appears in the sac; bubbles having
 483 sizes similar to the hole diameter appear in the hole. The simulation model
 484 predicts high velocities in the hole; however, since the flow coming from the
 485 seat is throttled a void structure appears in front of the hole. The bubbly
 486 mixture in the sac volume correlates to the void structure created in front of
 487 the hole, which is predicted to be composed of a mixture of fuel vapour and
 488 expanded air. On the other hand, the visualised bubbles computed inside
 489 the injection hole correlate to the big amount of cavitation computed in the
 490 hole.

491 A time sequence of the pressure field is presented in Figure 11. Before
 492 the needle valve closes, the predicted sac volume pressure is still higher than
 493 the ambient pressure ($t = 0.674ms$), but immediately after the needle valve
 494 closing ($t = 0.698ms$), a pressure wave is generated that travels towards the

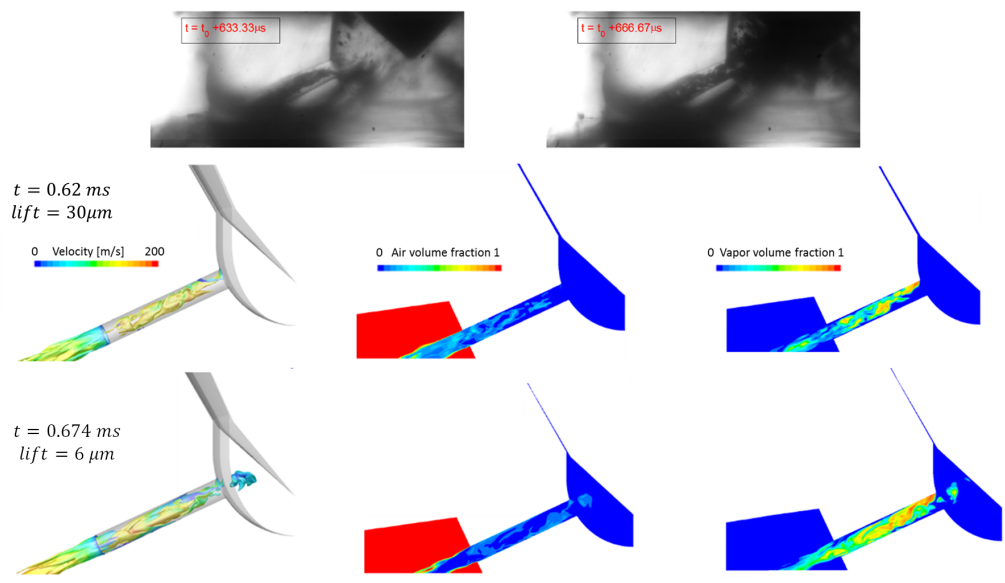


Figure 10: Needle closing results. Experimental visualisations for two time instants (top). Simulation results (center and bottom). For the simulation results 50% liquid volume fraction iso-surface coloured by velocity magnitude (left), air volume fraction contours (center) and vapour volume fraction contours (right) are presented.

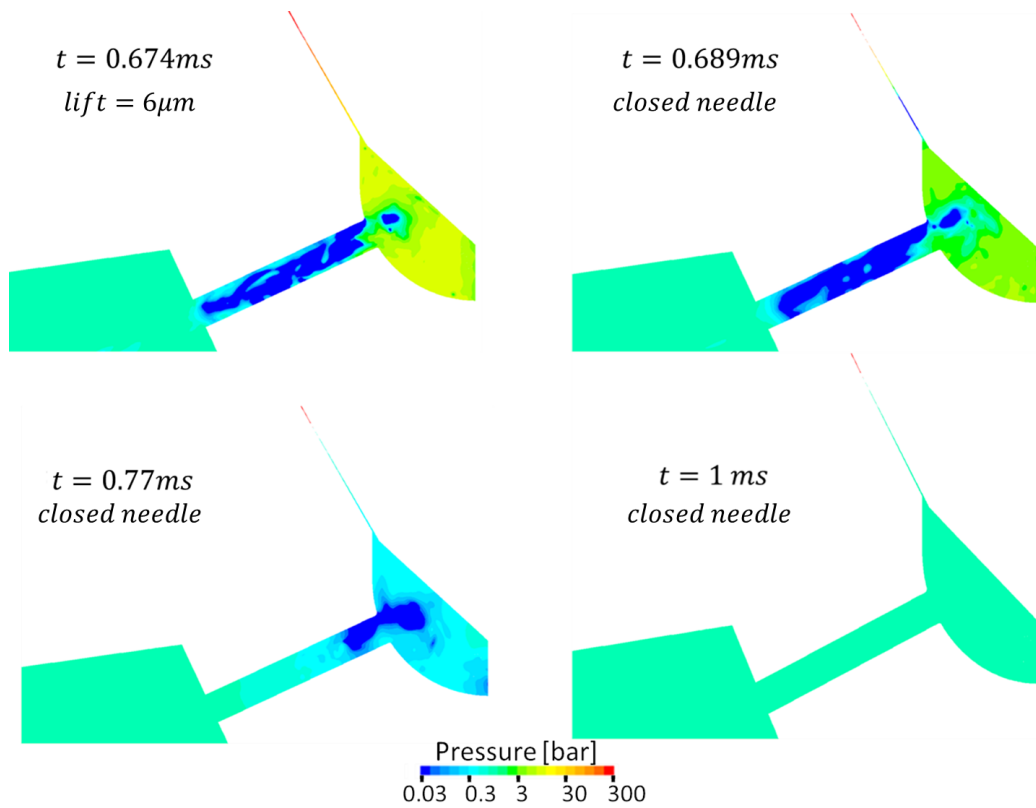


Figure 11: Pressure field time sequence. Notice that logarithmic scale has been used.

495 sac volume; this leaves the sac volume pressure below the ambient pressure
 496 ($t = 0.77ms$). In agreement with Figure 6, where air volume fraction inside
 497 the nozzle is seen to increase after needle closing, this induces the spray to
 498 weaken and air to be sucked back from the ambient into the nozzle until the
 499 sac pressure is balanced with the exterior pressure ($t = 1ms$).

500 Evidence is also provided in Figure 12, which shows a time sequence
 501 of air and vapour volume fraction fields. It clearly depicts the weakening
 502 flow momentum in the injection hole ($t = 0.698ms$) leading to air suction

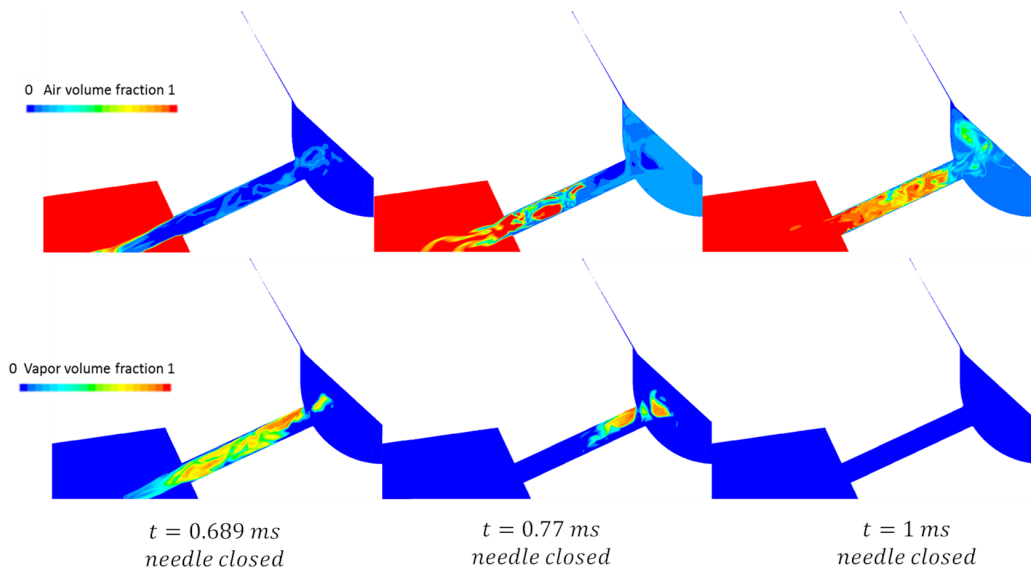


Figure 12: After needle closing results. Time sequence for air (top) and vapour (bottom) volume fraction fields.

503 ($t = 77ms$). Finally, due to the pressure balancing with the ambient pressure,
 504 vapour completely disappears ($t = 1ms$), indicating that shortly after the
 505 needle closing only liquid and air remain inside the sac volume.

506 5. Conclusions

507 This paper presents an investigation of cavitation and air interaction dur-
 508 ing a diesel pilot injection of a standard serial production six-hole geometry.
 509 The focus was to understand the complex interaction between the needle mo-
 510 tion, cavitation formation and development, and gas suction. The strategy
 511 followed has been to use high speed visualisations of a transparent nozzle
 512 tip to record the multiphase phenomena and to use CFD to explain the
 513 physics behind the observations. The CFD methodology includes LES tur-

514 bulence modelling, the needle valve movement, cavitation effects through a
515 Rayleigh-Plesset based cavitation model, and the compressibility of both air
516 and fuel. Starting from a flow field initialised according to the experimental
517 observations (with an air bubble in the sac and a big portion of the hole
518 filled with air), the main flow features observed are replicated by the simu-
519 lations. In particular the following phenomena experimentally noticed have
520 been explained and reproduced:

- 521 • The compression of the initial air bubble due to sac pressure build
522 up. The inclusion of air compressibility in the simulation can be very
523 relevant even for modest injection pressures in order to replicate the
524 air compression in the sac at the start of the injection as well as the
525 air expansion in the injection hole and sac.
- 526 • The appearance of cavitation stemming from the sac entry at the start
527 of the injection, due to flow separation and shear.
- 528 • The sac flow recirculation in the sac and flow patterns inside the hole.
529 One part of the void observed in the simulation can be attributed to
530 cavitation both geometrical (developed at the hole inlet upper lip) and
531 vortical (due to complex flow structure coming from the sac). Further-
532 more, the initial air inside the nozzle expands in the hole contributing
533 to the void areas observed. This shows that the void observed experi-
534 mentally is a combination of both air and fuel vapour.
- 535 • An increase of void inside the hole and in the sac during the needle

536 valve closing. The underlying reason being the flow throttling, since
537 liquid momentum is still high but flow passage very restricted.

538 • The air suction after the needle closing. The closure of the valve creates
539 an expansion wave that leaves the sac pressure below the ambient. This
540 induces vapour creation and air expansion in the sac and consequently
541 air is sucked from the ambient into the nozzle. When the pressure in
542 the sac is recovered, all vapour collapses. Therefore, it is shown that
543 the remaining foam at the end of the injection consists of a liquid and
544 air mixture.

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