

# Numerical and Experimental Investigation of Early Stage Diesel Sprays

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## Abstract

Experimental and numerical investigations of primary atomization in a high-pressure diesel jet are presented. Information on flow processes and structures inside and near nozzle exit are described at early and quasi-steady stages of injection. The numerical method is based on the Volume Of Fluid (VOF) phase-fraction interface capturing technique, in an Eulerian framework. The influence of grid resolution, convection interpolation scheme and temporal integration scheme on the modelling of jet physics are investigated. The present flow setup includes in-nozzle disturbances with the no-slip condition at the walls. All experimental operating conditions are replicated in the numerical models. The early stage liquid jet leading edge demonstrates an umbrella-shaped structure in the numerical results which is in qualitative agreement with experimental imaging. Data obtained provide insight into the flow behavior in the dense region including commencement of fragmentation and early spray angle formation. Experimental images show a cloud of air-fuel mixture at the early stage of injection. The existence of ingested air inside the injector after needle closure could be the source of the observed deviation between experimental and numerical results. The results show that the jet break-up rate and liquid core length increase in cases with higher grid resolutions. The early spray angle from the numerical results at the quasi-steady stage, shows good agreement with experimental data.

## Keywords

High-pressure diesel spray; Primary atomization; Near-nozzle flow; In-nozzle turbulence; Large Eddy Simulation; Eulerian/VOF.

## 24 1. Introduction

25 Steady and unsteady liquid jet flows and their breakup remain an ongoing field of investigation [1-8].  
26 Jets are of broad interest for the study of many basic phenomena and in a range of physical processes.  
27 They occur at length scales ranging from the order of atomic to that of the universe. In many applications,  
28 they may be multi-phase and involve multiple phase changes, chemical reactions and complex flow  
29 phenomena.

30 Human impacts on the environment and more specifically global warming are increasing government  
31 concerns on strict emission standards for engine manufacturers. The quality of air-fuel mixing is mainly  
32 driven by atomization of the injected liquid jet, which plays an important role in the combustion process,  
33 ultimately controlling production of pollutants. Engine manufacturers are constantly aiming to reduce  
34 exhaust gas emissions by optimizing the fuel injection process. A wide range of engine operating  
35 conditions makes the optimization of air-fuel mixing difficult [8-11]. The motivation, on one hand, is  
36 practical applications such as manufacturing of diesel engine injectors and, on the other hand,  
37 understanding the origin of key phenomena of atomization and its influence on jet breakup processes.

38 In diesel engines, combustion chambers are fed by high-pressure fuel injected as a solid cone spray.  
39 This spray undergoes a series of instabilities (longitudinal and transverse) which lead to the fragmentation  
40 of the liquid bulk into structures that further disintegrate into droplets. This initial process of atomization  
41 is called primary breakup and occurs in the vicinity of the injection point. Primary breakup mechanisms  
42 initiate the atomization process, control the extent of the liquid core and provide initial conditions for  
43 secondary breakup in the disperse flow region [5, 10, 12, 13].

44 Despite the fact that atomization is widely utilized and significantly affects engine combustion  
45 processes, heat release rate and exhaust emissions [2, 14-17], the characteristics of the spray produced

46 (for example size and velocity distributions of droplets) are still not well predicted due to the small length  
47 and time scales and high liquid fractions involved, especially inside the jet.

48 So far, many theories have been proposed to describe the primary atomization mechanism, including:  
49 aerodynamic shear forces which act through stripping and Kelvin-Helmholtz (K-H) instabilities [8, 18,  
50 19]. Turbulence-induced disintegration has a significant effect on jet breakup at higher Reynolds numbers  
51  $Re_l = \rho_l U D / \mu_l$ , where  $\rho_l$  is the liquid density,  $U$  is the liquid velocity,  $D$  is the orifice diameter, and  $\mu_l$  is  
52 the dynamic viscosity [14, 16, 20-23]. Relaxation of the velocity profile, creates a bursting effect  
53 especially in non-cavitating jets and large velocity differentials [24]. Cavitation-induces disintegration of  
54 the jet due to the reduction of cross-sectional area at the nozzle inlet [25-28]; and liquid bulk oscillation  
55 provoking toroidal surface perturbations [8, 29].

56 Less of a consensus has been achieved in determining the dominant mechanisms of early breakup  
57 when a high-speed liquid jet is injected into a pressurized dense gas. Many interdependent phenomena  
58 can provoke severe velocity fluctuations leading to a nonlinear instability of the flow inside the nozzle.  
59 These phenomena include turbulence [16, 20-23] generated by the nozzle geometry and by the collapse of  
60 cavitating bubbles [25-28]. In addition to turbulence, fluctuations of the injection velocity [24] and drop  
61 shedding [14, 30] contribute to the primary breakup. Experimentally separating and investigating these  
62 different effects is very difficult. For the development of diesel engines with both optimal fuel economy  
63 and minimum pollutant emissions, it is necessary to comprehend the spray processes and then  
64 characterize the effects of different parameters and engine operating condition on fuel flow structures.  
65 This is a challenging subject to study, both experimentally and numerically [4, 15, 18, 31, 32]. In this  
66 study, the flow inside the nozzle and the liquid bulk near the nozzle exit and its fragmentation (primary  
67 atomization) are investigated.

68 This paper concentrates on the effect of in-nozzle turbulence. The effects of cavitation will be studied  
69 in future work. Turbulent flows are represented by eddies with an entire range of length and time scales.  
70 Large eddy simulation (LES) directly resolves large scale eddies and models small eddies. Simulating  
71 only small eddies and solving the large eddies allows the use of much coarser meshes and longer time  
72 steps in LES compared to Direct Numerical Simulation (DNS). Despite this, LES still needs principally  
73 finer meshes compared to the ones used for Reynolds Averaged Navier Stokes (RANS) computations.  
74 Since RANS models cannot capture the transient spray structure [5, 6, 8, 9] including droplet clustering  
75 and shot to shot variability, LES is applied to overcome these limitations.

76 Literature reviews of the existing atomization models, demonstrated that all these models (blob,  
77 Huh/Gosman, MPI, Arcoumanis, Nishimura, V.Berg, Baumgarten, ReitzWave model, Taylor Analogy  
78 Breakup model) [9, 32, 33] simplify droplet generation in the dense region (primary atomization) which  
79 might make the simulation inaccurate and unrealistic [6, 18]. For example, the blob model as the most  
80 employed model not only simply generates parcels with the size of the nozzle diameter but also does not  
81 take into account the physics of in-nozzle turbulence and in-nozzle cavitation. In addition, these  
82 conventional atomization models with Lagrangian Particle Tracking (LPT), limit the grid fineness near  
83 the nozzle and do not allow LES to capture the features of the spray and background fluid flow near the  
84 nozzle. Furthermore, refining the grid with the blob method results in problems with high liquid fraction  
85 in the LPT approach (too much liquid in each cell) [5, 6, 9, 34]. These limitations motivate the use of the  
86 Eulerian approach to model the primary atomization, instead of using conventional atomization models.  
87 With ever increasing computational power, there is an incentive to use more complex models for primary  
88 atomization. This is a key aim of the present work.

89 To date, considerable progress has been made in the development of rigorous numerical methods for  
90 performing highly resolved simulations of multiphase flow [8, 35]. The accuracy of different numerical  
91 techniques for modelling the primary atomization of a liquid diesel jet was investigated in detail for low

92 Re ( $Re < 5000$ ) by Herrmann [20] and Desjardins & Pitsch [36]. Herrmann [20], demonstrated the  
93 importance of the grid resolution on capturing the accurate phase interface geometry of diesel liquid with  
94 an injection velocity of 100 m / s and  $Re = 5000$ . Turbulence was reported as the dominant driving  
95 mechanism of atomization within the first 20 nozzle diameters downstream.

96 Due to the lack of detailed studies of the primary atomization of diesel liquid jets under real diesel  
97 engine operating conditions, the present study focuses on the structure of primary atomization with an  
98 accelerating injection pressure up to 1200 bar, background pressure of 30 bar, liquid Reynolds number  
99 within the range  $7000 \leq Re_l \leq 37000$ , and liquid Weber number of  $We_l \approx 933843$  at quasi-steady stage.  
100 The liquid Weber number  $We_l = \rho_l U_p d / \sigma$ , where  $U_p$  is the droplet relative velocity,  $d$  is the droplet  
101 diameter and  $\sigma$  is the surface tension. The Reynolds number is calculated based on average liquid velocity  
102 at the nozzle hole exit. The large range of  $Re$  is due to rising pressure at the sac inlet, changing from 30  
103 bar at the beginning of injection up to 1200 bar at the quasi-steady stage of injection. In-nozzle cavitation  
104 is not considered in this work however this constraint will be eliminated in further studies. The present  
105 work focuses on the very early stages of injection as it is likely that instabilities generated in the early  
106 stages have significant effect on the development of the whole spray. Non-evaporating conditions are  
107 employed to simplify the physical complexities.

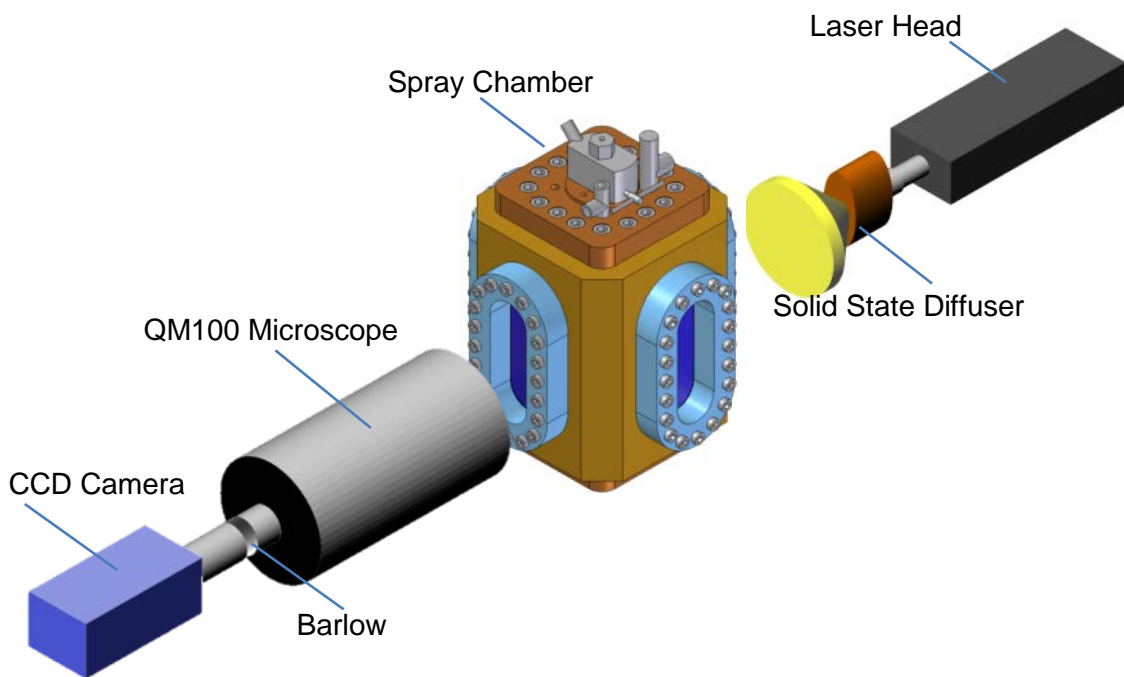
## 108 2. Methodology

### 109 2.1 Experimental apparatus

110 Non-evaporating diesel fuel spray measurements were conducted with a laser based imaging system  
111 in a constant volume High-Pressure Spray Chamber (HPSC). The HPSC operating volume is a square-  
112 section prism with rounded corners and the axis vertically oriented. Optical access to the injection test  
113 chamber is via three windows in the test chamber walls 80 mm thick, UV quality, optically polished

114 quartz, and viewing area of  $200 \times 70$  mm. The light source is a 120 milliJoule dual-cavity Nd:YAG laser  
115 capable of light pulses around 5 ns duration.

116 The chamber is pressurized to 30 bar with temperature and density of 298 K and  $35 \text{ kg/m}^3$ ,  
117 respectively, to give air density in the range of a heavy duty diesel engine. Diesel fuel is axially injected  
118 through a single solid cone fuel nozzle with an injection pressure of around 1200 bar from the top of the  
119 HPSC as shown in Figure 1.



120

121 **Figure 1.** Schematic view of the High-Pressure Spray Chamber showing laser and camera setup for  
122 shadowgraphy measurements.

123 The injection pressure profile which is highly repeatable from shot to shot is replicated based on the  
124 previous study of Bong et al [9]. The injector needle valve snaps open when the injector pressure achieves  
125 a given value, as determined by the tension of the needle valve spring. Needle lift is monitored using an  
126 eddy current proximity probe. It takes about 0.2 ms for the needle valve to lift completely.

127 The acquisition sequence is triggered by a pulse from the injector driver and the delay to the start of  
128 image acquisition is measured separately. The needle lift signal and the pulse generated by the laser were  
129 recorded using a digital oscilloscope to record the time at which the laser light pulse is activated, as  
130 indicated by the Q-switch pulse. Using shots obtained at the point where the spray is just starting to  
131 emerge from the nozzle, it is established that there is a delay of  $100 \pm 5 \mu\text{s}$  between start of injection and  
132 a significant response from the needle lift transducer. This information enables timing of subsequent  
133 shots.

134 A laser-based backlit imaging method (shadowgraphy) is used to investigate the micro-spray  
135 structure. As depicted in Figure 1, a Questar QM100 long distance microscope is attached to a LaVision  
136 Imager Intense dual-frame, 12 bit CCD camera with  $1376 \times 1040$  pixels. The camera and laser allow only  
137 two images to be taken for each shot of the injector. The delay between the two images can be as low as  
138  $0.5 \mu\text{s}$ . The use of closely spaced images allows estimation of the propagation velocity of the leading  
139 edge of the injected fuel. An interval of about 30 s is allowed between injector shots to allow the chamber  
140 to settle.

141 The spray is backlit with laser light through a standard solid-state diffuser supplied by LaVision. The  
142 diffuser employs laser-induced fluorescent from an opaque plate impregnated with a fluorescent dye. The  
143 camera is focused, aligned, and calibrated on a graduated scale on the spray axis.

144 Two sets of microscopic data are achieved with and without using a Barlow lens. With the 2x Barlow  
145 lens, mounted between CCD Camera and Microscope, a magnification of 7.7:1, a field of view of  
146  $1157 \times 860 \mu\text{m}$  and a spatial resolution of  $0.84 \mu\text{m}/\text{pixel}$  are achieved. These sets of data are used as a  
147 benchmark to validate the numerical results close to the nozzle exit.

## 148 2.2 Simulation setup

### 149 2.2.1 Mathematical method

150 In this study, the VOF phase-fraction based interface capturing technique similar to de Villiers et al  
151 [11] is employed in the open source numerical code OpenFOAM v2.3. The code considers the two-phase  
152 flow field as a single incompressible continuum with constant density  $\rho$  and viscosity  $\mu$ , including surface  
153 tension. The compressibility effect will be included in future studies. The basic form of the governing  
154 mass and momentum conservation are:

$$\nabla \cdot \mathbf{V} = 0 \quad (1)$$

$$\frac{\partial \rho \mathbf{V}}{\partial t} + \nabla \cdot (\rho \mathbf{V} \mathbf{V}) = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \int_{S(t)} \sigma \kappa' \mathbf{n}' \delta(x - x') dS \quad (2)$$

155 Where  $\mathbf{V}$  is the velocity,  $p$  is the pressure,  $t$  is the time,  $\boldsymbol{\tau}$  is the stress tensor,  $\kappa$  is the local curvature  
156 of the liquid surface and,  $\mathbf{n}$  denotes a unit vector normal to the liquid surface  $S$ . The operators  $\nabla(\cdot)$  and  
157  $\nabla \cdot (\cdot)$  represent the gradient and the divergence operations, respectively. The integral term in equation (2)  
158 represents the momentum source due to surface tension force on the interface  $S(t)$ . This force only acts on  
159  $S$ , as ensured by the indicator function  $\delta(\dots)$ . The time-varying phases interface  $S(t)$  is located  
160 accordingly using a VOF surface-capturing approach which utilizes the volume fraction  $\gamma$  of diesel fuel as  
161 an indicator function, defined as:

$$\gamma = \begin{cases} 1 & \text{for a point inside the liquid} \\ 0 < \gamma < 1 & \text{for a point in the transitional region} \\ 0 & \text{for a point inside the air} \end{cases} \quad (3)$$

162 The ‘transitional region’, where the interface is located, utilized as an artefact of the numerical  
163 solution process. Fluid in a transition region is considered as a mixture of the two fluids on each side of  
164 the interface, which cannot completely resolve a discontinuous step. The transport equation for the  
165 indicator function is:



$$\frac{\partial \gamma}{\partial t} + \nabla \cdot (V\gamma) = 0 \quad (4)$$

166 According to the definitions of  $\gamma$ , the local thermo-physical properties are given by:

$$\rho = \gamma\rho_l + (1 - \gamma)\rho_g \quad (5)$$

$$\mu = \gamma\mu_l + (1 - \gamma)\mu_g \quad (6)$$

167 where the subscripts  $l$  and  $g$  represents the liquid and gas, phases respectively.

168 The LES/VOF equations are derived from equations (1), (2) and (4) using localized volume  
 169 averaging of the phase-weighted hydrodynamics variables. This process known as filtering, includes  
 170 decomposition of the relevant variables into resolvable and sub-grid scales of turbulent fluctuations. As  
 171 the results of the filtering process, the sub-grid scale fluctuations will be eliminated from direct  
 172 simulation. This filtering together with the non-linear convection terms in equation (2) introduce an  
 173 additional quantity, comprising correlation of the variable fluctuations at sub-grid scales that entail  
 174 closure through mathematical models, known as the subgrid scale (SGS) stresses  $\tau^{sgs}$  as they signify the  
 175 influence of the unresolved small scales of turbulence, given by:

$$\tau^{sgs} = \overline{V\overline{V}} - \overline{V}\overline{V} \quad (7)$$

176 and estimated by a single subgrid scale model of the eddy-viscosity type:

$$\tau^{sgs} - \frac{2}{3} k \mathbf{I} = - \frac{\mu^{sgs}}{\rho} (\nabla \overline{V} + \nabla \overline{V}^T) \quad (8)$$

177 where  $k$  is the subgrid scale turbulent energy and  $\mu^{sgs}$  is the subgrid scale viscosity, both are determined  
 178 from the one-equation SGS turbulent energy transport model accredited to Yoshizawa [37].

$$\frac{\partial k}{\partial t} + \nabla \cdot (k\overline{V}) = \nabla \cdot [(v + v^{sgs})\nabla k + \tau^{sgs} \cdot \overline{V}] - \varepsilon - \frac{1}{2} \tau^{sgs} : (\nabla \overline{V} + \nabla \overline{V}^T) \quad (9)$$

179 where  $\varepsilon = C_\varepsilon k^{2/3}/\Delta$  is the SGS turbulent dissipation rate,  $\nu^{sgs} = C_k k^{1/2}/\Delta$  and  $\Delta = \sqrt[3]{V}$  is the SGS  
180 length scale where  $V$  is volume of the computational cell. The coefficients, found from statistical  
181 considerations, are  $C_k = 0.05$  and  $C_\varepsilon = 1$  [6].

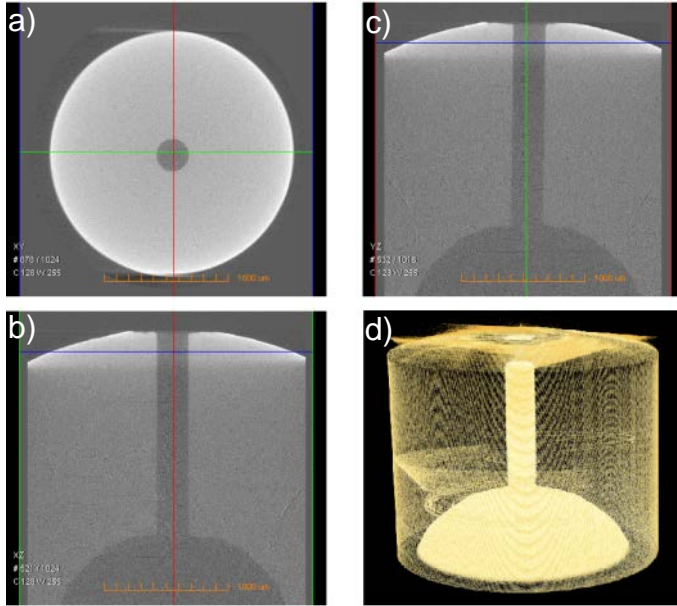
### 182 2.2.2 The Numerical solution method

183 Mathematical models for this simulation are solved using an implicit finite-volume method, which  
184 employs spatial and temporal discretization schemes. This method preserves a sharp interface resolution  
185 by including a compression velocity term [38] in the phase transport equation, acting to compress the  
186 VOF interface. The solution procedure utilizes the Pressure Implicit with Split Operator (PISO) algorithm  
187 [39], together with conjugate gradient methods for coupled solution of mass and momentum conservation  
188 equations which is specifically suited to transient flows [40].

189 In order to preserve the proper physical limits on the fluid-dynamics variables, different integration  
190 schemes are tried from highly dissipative up to highly conservative. In this study, the advection terms are  
191 solved by the Normalized Variable (NV) Gamma differencing scheme [41]. A conservative, bounded,  
192 second-order scheme is used for Laplacian derivative terms and a second-order, implicit discretization  
193 scheme is used for time derivative terms. The numerical integration time-step is adjusted by various  
194 stability criteria, and is of the order  $1 \times 10^{-9}$  s for the fine case.

### 195 2.2.3 Boundary conditions and initial setup

196 Atomization is affected by the design of the sac and nozzle orifice inlet which consequently influence  
197 primary breakup [8, 14, 18]. The computational domain has therefore been modelled using the geometry  
198 of the experimental nozzle determined using X-ray Computer Aided Tomography (CAT) analysis as  
199 shown in Figure 2. This analysis reconstructs the images with pixel numbers of  $1016 \times 1024 \times 1024$ , and  
200 effective voxel size of  $2.318 \mu\text{m}$ .



201

202 **Figure 2.** X-Ray Tomography measurement of sac and nozzle geometry and dimensions. a) X-Y view;  
 203 b) X-Z view; c) Y-Z view and d) 3D view of nozzle. Images provided by The Centre for Materials and  
 204 Surface Science and the Centre of Excellence for Coherent X-ray Science at La Trobe University,  
 205 employing an Xradia MicroXCT instrument.

206 All the experimental conditions were replicated in numerical models including the sac volume inlet,  
 207 spray chamber pressure and air and diesel fuel temperature and viscosity. Fuel properties and set up  
 208 conditions are listed in Table 1. The sac inlet pressure is ramped from 30 bar initially to 850 bar after 50  
 209  $\mu\text{s}$  then to 1200 bar after a further 25  $\mu\text{s}$  then constant at 1200 bar to the end of simulation. This is to  
 210 some extent arbitrary but is premised on published data implying that the sac pressure rises rapidly during  
 211 needle opening [1, 42-44]. For instance, Moon et al. [1] found that quasi-steady stage jet velocity was  
 212 reached when the needle lift was only 17% of the maximum needle lift. The ramp was chosen to give an  
 213 approximate match of modelled and experimental penetration rates. The lower pressure rise rate in the  
 214 second 25  $\mu\text{s}$  was adopted to avoid numerical instabilities.

215 In the present study, it was found that the duration of the needle lift is about 200  $\mu\text{s}$  and that the  
 216 signal from the eddy current needle lift transducer signal has a delay of around  $100 \pm 5 \mu\text{s}$  compared to  
 217 actual needle lift. This is determined by observing the timing of the laser Q-switch signal relative to the

218 needle lift signal for shots where the captured image shows the spray just starting to emerge from the  
 219 nozzle. Thus, the needle lift signal could not be used to determine instantaneous needle position. The  
 220 maximum needle lift is about 200  $\mu\text{m}$ .

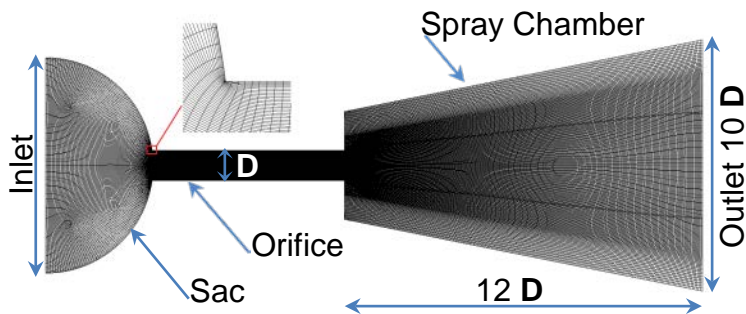
221 **Table 1.** Fuel properties and operating conditions based on experimental setup [45]. \* Injection velocity,  
 222 Weber and Mach numbers are for the quasi-steady stage of spray [45]. The nozzle diameter is used as the  
 223 length scale.

Parameter	Value
Injection pressure	120 MPa average
Nozzle diameter	0.25 mm
Nozzle length	1.6 mm
Nozzle nominal geometry	$K_s = 0$
Fuel	Diesel
Diesel fuel density	832 kg/m <sup>3</sup>
Gas	Compressed air
Density ratio	42
Fuel Kinematic viscosity	$2.52 \times 10^{-6} \text{ m}^2/\text{s}$
Surface tension	0.03 N/m
Temperature	25°C
Fuel $Re_1$	$7000 \leq Re \leq 37000$
*Indicative injection velocity	367
*Fuel Mach number	$367 / 1250 = 0.3$
* $We_1$	933843
*Ohnesorge number	0.077
Chamber pressure	30 bar

224 The nozzle orifice at the start of each injection in the experimental injections is not necessarily full of  
 225 fuel due to needle bounce and dribble phenomena at closure nor empty of fuel due to cohesive and  
 226 adhesive forces. Hence for a good comparison of modelled and measured injection, a method for  
 227 determining the position of the liquid-gas interface in the nozzle orifice at the start of injection was  
 228 implemented. Firstly, the sac and three quarters of the nozzle were filled with diesel fuel at a pressure of  
 229 30 bar and then the sac inlet pressure raised as described above. Later on, at the end of the injection cycle  
 230 when the needle closes, the boundary condition is changed from inlet to wall to prevent any further fuel  
 231 entering the sac, emulating the needle valve closure process. The result of this simulation is that the

232 nozzle fills with liquid to 5.2 D (81% of the nozzle length) from the nozzle entrance. This is due to the  
 233 equilibrium between adhesive forces, surface tension of the liquid phase and hydrodynamic forces  
 234 amongst liquid and pressurized air in the spray chamber. The position of the liquid-gas interface inside  
 235 the nozzle orifice resulting from this simulation (at 5.2 D) is used to initialize the main simulation. This  
 236 starting point is somewhat arbitrary but goes some way to accounting for air ingestion as described in  
 237 [42-44, 46].

238 Considering the boundary layer, atomization zone and no-slip condition at the walls (sac and orifice),  
 239 a hexahedral structured mesh was generated as shown in Figure 3. It has been reported that the spray  
 240 structure is not axisymmetric [5, 9, 14, 34, 45], therefore the full computational domain ( $360^\circ$ ) of the  
 241 atomization zone is meshed.



**Figure 3.** Computational domain and boundary conditions (coarse case, with refined mesh in the orifice and atomization regions).

243 In order to conduct a mesh sensitivity study, three different mesh resolutions are generated with  
 244 coarse (4 million cells), medium (8 million cells), and fine grids (20 million cells). Cell size is refined  
 245 down to  $0.1 \mu\text{m}$  in the orifice and  $1.7 \mu\text{m}$  in the primary atomization zone in the finest resolution case.  
 246 This cell size can capture droplets down to the  $10 \mu\text{m}$  range based the optimistic premise that 5 cells can  
 247 give reasonable representation of a single droplet [20]. The resolution of these cases, time-step range,  
 248 number of CPUs, and computational cost (wall clock time) for each case are summarized in Table 2.

249 **Table 2.** Summary of mesh parameters for numerical models

Case	Average Resolution ( $\mu\text{m}$ )			Cell count	Time Step ( $\times 10^{-9}$ S)	CPU (core count)	Wall clock time (hours)
	Sac	Orifice	Spray Chamber				
Coarse	13	2	6.5	$4 \times 10^6$	$1.6 \leq \Delta T \leq 80$	128	151.4
Medium	7.5	1.2	5	$8 \times 10^6$	$1.2 \leq \Delta T \leq 60$	256	225.8
Fine	4	0.5	3.5	$20 \times 10^6$	$0.9 \leq \Delta T \leq 30$	384	565.3

250 Being aware of the importance of in-nozzle generated turbulence on primary atomization [18, 20], in  
251 the fine case, special consideration was given to generating the mesh inside the nozzle orifice. The size of  
252 cells in the orifice were decreased to the order of the Kolmogorov length scale for the liquid phase,  $\eta_l$ , to  
253 assure that the smallest generated eddies, as a result of boundary layer and change in cross sectional area,  
254 are well resolved. The smallest length scales associated with the flow field for the quasi-steady stage of  
255 spray are reported in Table 3. It can be seen in this table that  $\eta_l$  is much larger than mesh size in the  
256 nozzle for the finest grid. To resolve a given length scale it is necessary that  $\eta_l \geq 2\Delta x$ , where  $\Delta x$  is the  
257 grid size [41]. This mesh resolution leads to the proper prediction of small eddies of the liquid phase  
258 inside the nozzle orifice in the fine resolution case. A sub-grid scale model is needed for the turbulence in  
259 the gas phase.

260 **Table 3.** Kolmogorov length scales for the liquid and gas phases of the quasi-steady stage of spray where  
261 the turbulence intensities used are 4.4 % and 10 %, respectively.

Parameter	Value
Liquid phase Kolmogorov length scale, $\eta_{\text{liq}}$	0.7 $\mu\text{m}$
Minimum mesh size in nozzle hole for fine case, $\Delta x_{\text{min}}$	0.1 $\mu\text{m}$
Gas phase Kolmogorov length scale, $\eta_{\text{gas}}$	0.008 $\mu\text{m}$
Minimum mesh size in spray chamber for fine case, $\Delta x_{\text{min}}$	1.7 $\mu\text{m}$

## 262 2.2.4 Mesh sensitivities

263 In this research structured grids are used to achieve higher quality and control which may be  
264 sacrificed in unstructured and hybrid meshes. In addition, the efficiency of the differencing scheme for

265 bounding the convection term of the transport equations in a structured mesh is much higher in  
266 comparison to an unstructured mesh [47].

267 It is possible that the present conically stretched grid leads to greater spray angle than a purely  
268 Cartesian/orthogonal grid, for example. The core of the mesh is purely Cartesian/orthogonal, and the  
269 divergence immediately adjacent to the core region is less than near the outer boundaries. Using a  
270 structured mesh as in the present study reduces the effects of divergence from orthogonality. A non-  
271 orthogonality corrector is employed in the numerical solution to minimize any possible grid orientation  
272 influences.

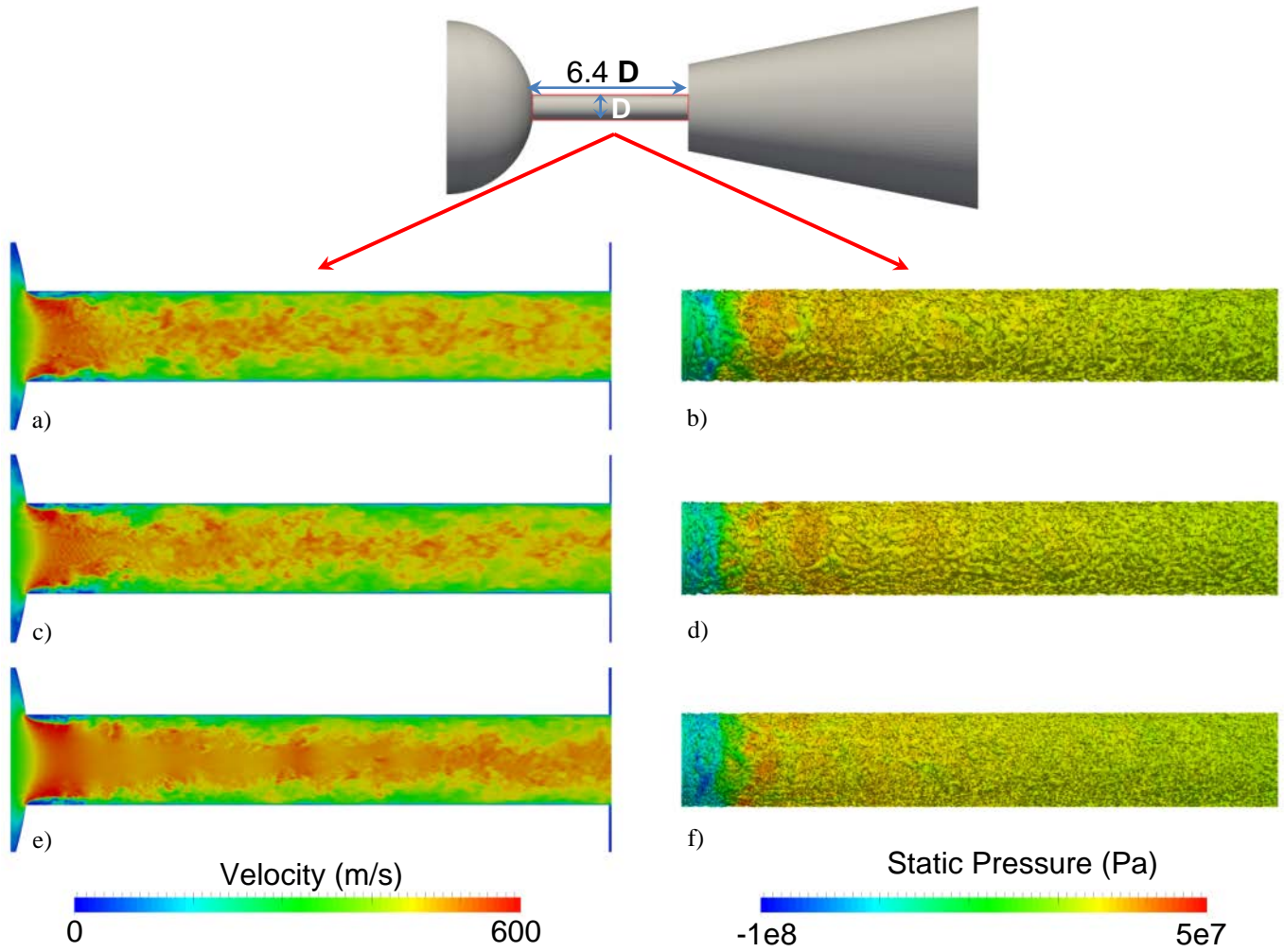
### 273 **3. Results and discussions**

274 Due to the unavailability of a transparent orifice, only images of the spray in the chamber are  
275 presented. The comparisons between simulations and experiments are qualitative and focus on the overall  
276 spray shape, surface irregularities, spray penetration and generated droplets. The numerical data presented  
277 in the next two sections are obtained by means of the second-order time derivatives method and the NV  
278 Gamma scheme for solving the convection terms.

#### 279 **3.1 In-nozzle turbulence**

280 Figure 4 illustrates the influence of mesh resolution on turbulent eddies, generated and developed  
281 within the orifice boundary layer leading to small/large-scale irregularities. These irregularities are the  
282 origin of jet surface instabilities. This Figure shows a zoomed view of the jet turbulent structures inside  
283 the nozzle orifice demonstrating the small-scale eddies in each case at the quasi-steady stage (sac inlet  
284 pressure of 1200 bar and Re of 37000 at the orifice exit). In the left column (images *a*, *c*, and *e*), in-nozzle  
285 flow is coloured by velocity magnitude. In the right column at corresponding times (images *b*, *d*, and *f*),  
286 the turbulent eddies are depicted using a Q-criterion isosurface of  $5 \times 10^9$ , coloured by static pressure.  
287 Negative static pressures after the nozzle entrance are due to the absence of a cavitation model. In the

288 high-resolution case, smaller eddies have been resolved demonstrating the importance of mesh resolution  
 289 on predicting upstream flow conditions.



291 **Figure 4.** Jet liquid turbulent structures at quasi-steady stage ( $P_{inlet} = 1200$  bar and  $Re = 37000$  at the  
 292 orifice exit for coarse (a and b), medium (c and d) and fine (e and f) mesh cases. In the left column  
 293 (images a, c, and e), in-nozzle flow is coloured by velocity magnitude. In the right column at  
 294 corresponding times (images b, d, and f), the turbulent eddies are illustrated using a Q-criterion isosurface  
 295 of  $5 \times 10^9$ , coloured by static pressure. Negative static pressures after the nozzle entrance are due to the  
 296 absence of a cavitation model. Greater resolution of jet core and boundary layer turbulence are apparent  
 297 with increasing mesh density.

### 298 3.2 Morphology of the penetrating jet

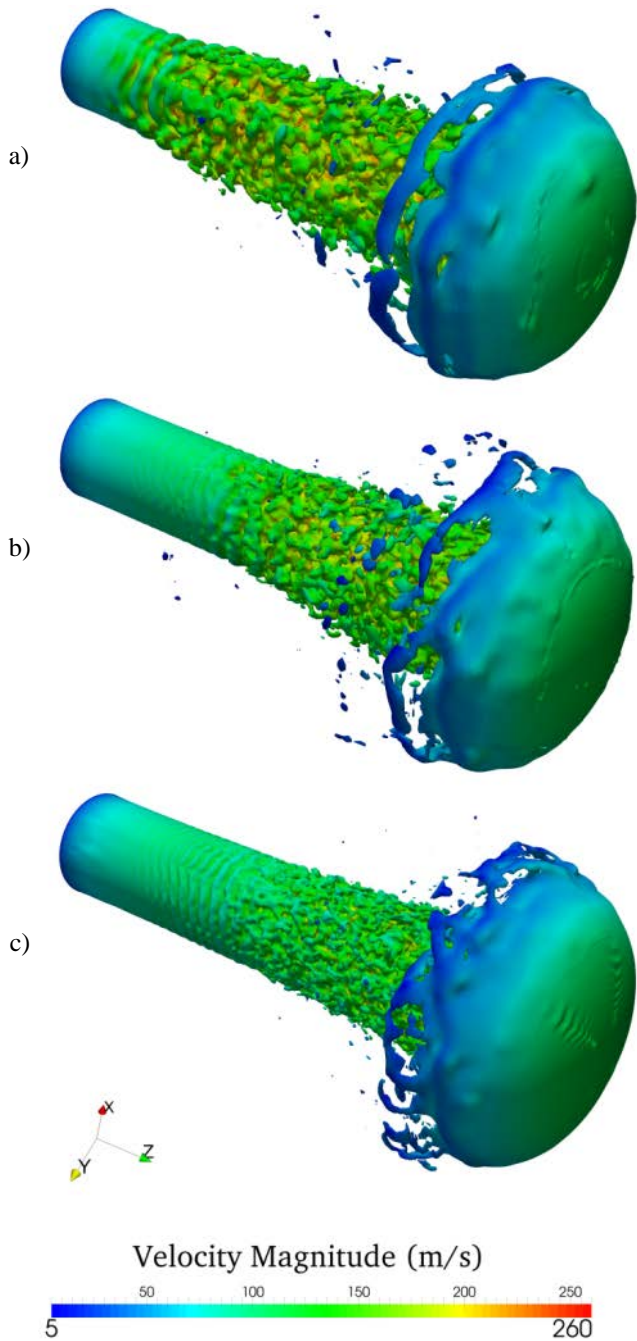
299 Some instantaneous features such as flow structures and the evolution of spray transients are  
 300 presented in Figure 5 for three different mesh resolutions at  $15 \mu s$  after start of penetration (ASOP)



301 showing the influence of mesh size on capturing surface instabilities. The umbrella-shaped leading edge  
302 of the jet for coarse, medium, and fine cases shows a smooth surface with penetration velocity of 123 m/s  
303 in agreement with DNS results [14, 34] for similar velocity ranges.

304 The irregularities on the trailing edge of the umbrella play a significant role in the disintegration  
305 process of the penetrating jet. As can be seen in Figure 5, finer grids lead to capturing more waves  
306 resulting in higher fragmentation rates.

307 Mesh resolution affects prediction of instabilities on the liquid jet behind the umbrella. In-nozzle-  
308 generated turbulence in combination with relaxation of the velocity profile at the nozzle exit initiate the  
309 perturbations leading to wave growth on the jet surface. As can be seen in Figure 5, surface instabilities  
310 are triggered close to the nozzle orifice exit (further than one diameter for the fine grid) as a result of the  
311 K-H mechanism (wave generation on jet surface based on aerodynamic interaction, creating ligaments  
312 which then either disintegrate to produce droplets or just roll up and continue to develop).



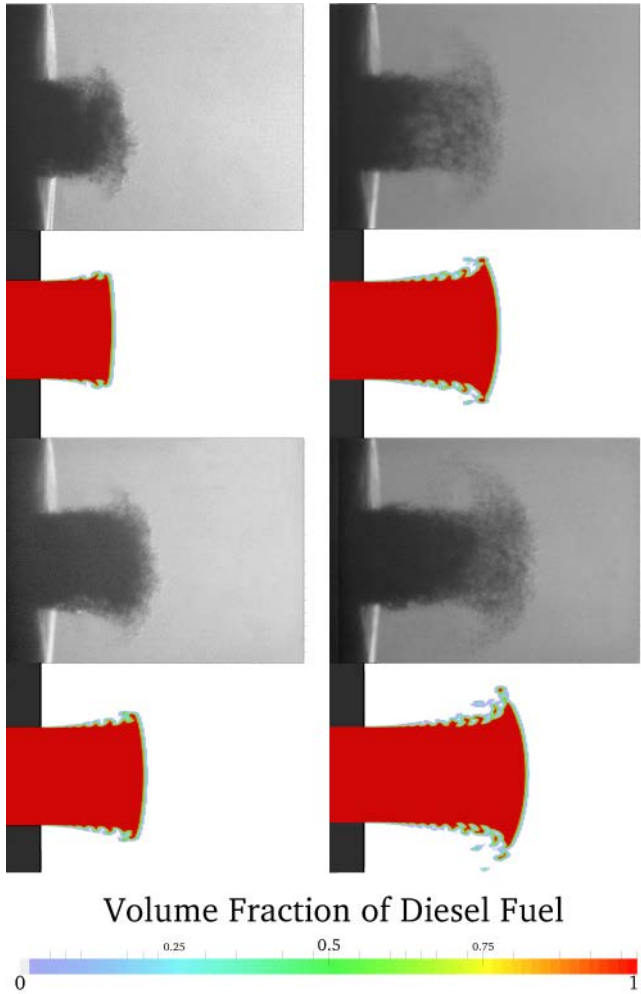
313

314 **Figure 5.** Structure of the jet colored by velocity magnitude at  $15 \mu\text{s}$  ASOP, indicated by liquid interface  
 315 of  $\gamma = 0.5$ , for coarse (a), medium (b) and fine (c) mesh cases showing over-prediction of breakup for the  
 316 coarse case and the resolution of smaller scale surface instabilities and breakup for the finer case.

317 Inaccurate prediction of the velocity relaxation at the liquid-gas interface due to insufficient grid  
 318 resolution intensifies the K-H mechanism, exaggerating the liquid jet disintegration process. Furthermore,  
 319 the thickness of ligaments is a matter of the cell size where the pinching-off occurs as the thickness drops

320 below the cell size, followed by the generation of several droplets of varying sizes [8, 48, 49]. It can be  
321 concluded that the mesh density at the air-fuel interface considerably influences the development of  
322 ligaments and the breakup process.

323 Figure 6 shows a comparison of experimental images with the numerical results with the fine mesh  
324 case at different times ASOP. Adding a 2× Barlow lens to the microscope to give a total magnification of  
325 7.7:1 enables greater details of the early spray to be captured. The use of a dual frame CCD camera with a  
326 time interval of one microsecond between subsequent images allows validation of the velocity of advance  
327 of the leading edge and tracking of the transient changes in the morphology of the penetrating diesel jet.



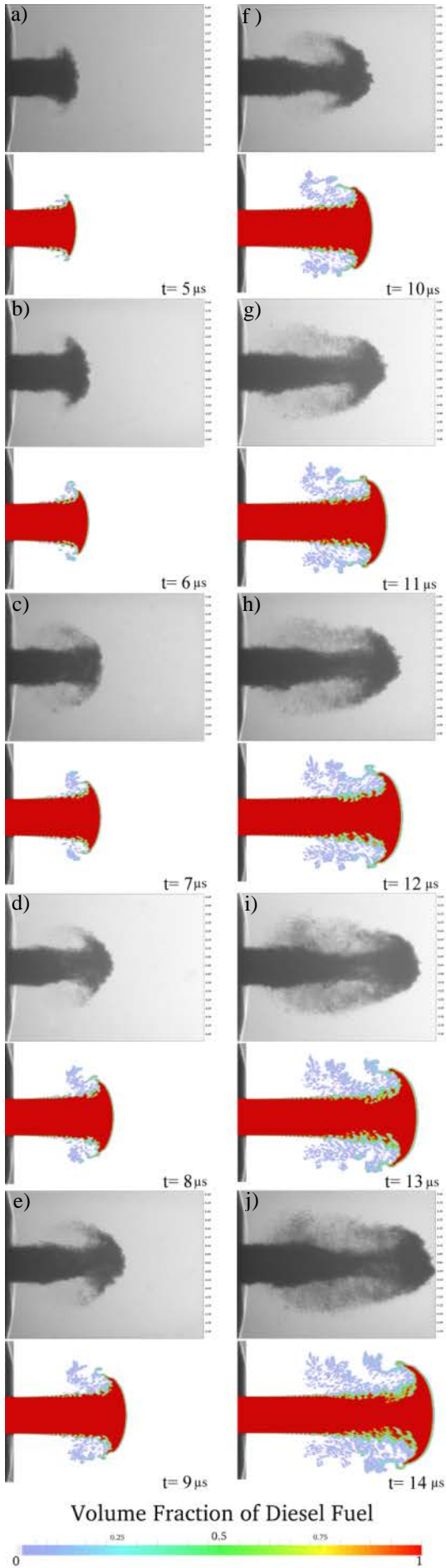
329 **Figure 6.** Comparison of experimental images with numerical results for the fine mesh case with highest  
330 magnification. Each experimental image is from a different injection event, apart from the first two  
331 (a and b) which are captured from two consecutive frames with 1  $\mu$ s inter frame time.

332 Some transparency can be clearly seen in the shadowgraphy images. This is due to air inclusion  
333 within the liquid inside the orifice, left from previous injection. The existence of ingested air inside the  
334 injector was reported by Swantek et al. [46] at the end of injection (EOI) process. Air inclusion inside the  
335 injector influences the spray structure and could be a source of observed deviation between experimental  
336 and numerical results.

337 Shadowgraphy images are compared with the numerical results in Figure 7 with a larger field of  
338 view, presenting the general structure of the diesel spray. In this Figure, images *a* and *b*, *d* and *e*, *g* and *h*,  
339 *i* and *j* are paired, each pair is captured from the same injection event with one microsecond delay  
340 between consecutive frames.

341 The experimental images illustrate a more structured surface even very close to the nozzle exit  
342 compared with the numerical results. The leading edge of the emerging jet is disintegrating unlike the  
343 numerical results where the leading edge umbrella-shaped structure of the emerging jet is continuous  
344 liquid with breakup occurring more rapidly around the periphery. Air inclusion prior to start of injection  
345 could explain the rougher surface, and earlier disintegration of the leading edge in the experimental  
346 images resulting in the more oblique angle of the umbrella.

347 The necking of the jet length behind the umbrella can be obviously seen in the experimental images  
348 in Figure 7, while it is not as marked in the simulations. The difference is possibly related to the presence  
349 of air in the experimental jet, as indicated by partial transparency of the experimental images, and thus  
350 more rapid disintegration. The outer recirculating gas flow removes the generated droplets and advects  
351 them toward the outer flow which can be seen in images *i* and *j* of Figure 7.

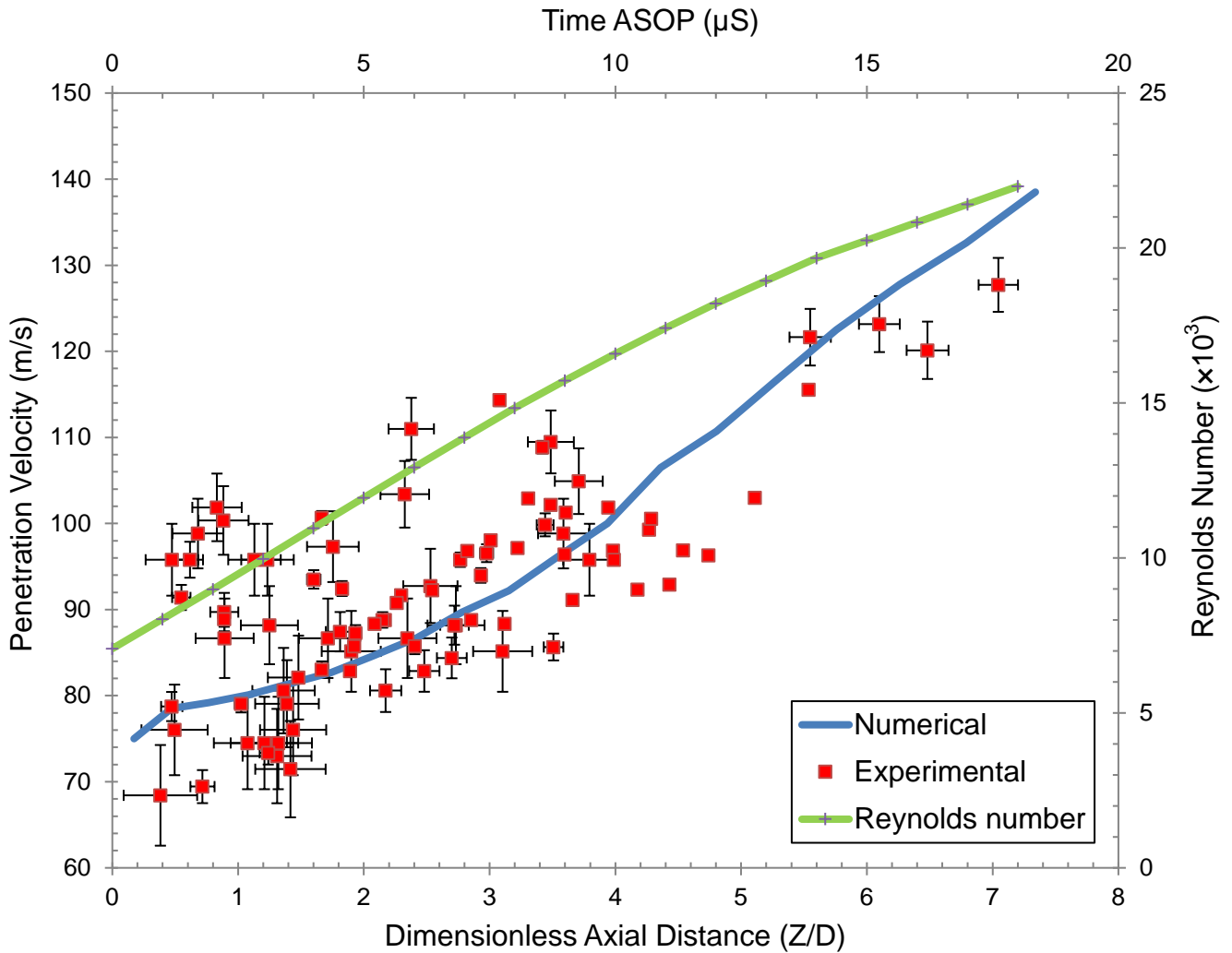


353 **Figure 7.** Comparison of experimental (with no magnification) and numerical results. Numerical results  
354 shown are for the fine mesh, colored by volume fraction of diesel fuel. Images a and b, d and e, g and h, i  
355 and j are paired, captured from the same injection event from two consecutive frames with  $1\ \mu\text{s}$  inter  
356 frame time.

357 Further differences between the experimental and numerical results are in the production of small  
358 droplets in the experimental images but not in the numerical results. This is due to the constraint in  
359 computational resources where the grid resolution in the computational domain is insufficient to resolve  
360 the small eddies in the air phase which influences the breakup processes of the ligaments and droplets.

361 Capturing two subsequent images enables velocity measurement of the jet leading edge.  
362 Experimental values for 100 double frame shots, with inter-frame times varying between 1 to  $15\ \mu\text{s}$  are  
363 shown in Figure 8. The error bars are based on the accuracy of the detection of the leading edge of the jet  
364 and this is a function of the inter-frame time. The jet penetration velocity at various axial distances from  
365 nozzle exit with corresponding time ASOP, demonstrated in Figure 8, show good agreement between  
366 numerical and experimental results. The  $Re$  is based on the average axial velocity at the nozzle exit.

367 Instantaneous mass flow rate was not measured. Quasi-steady mass flow rate was measured at  
368  $0.0139\ \text{kg/s}$  and numerically predicted at  $0.0168\ \text{kg/s}$ . The difference is assumed to be due primarily to  
369 the absence of cavitation in the simulations.



370

371 **Figure 8.** Comparison of measured and predicted jet penetration velocity at various axial distances from  
 372 nozzle exit with corresponding times ASOP. Re values, from computation, are calculated using the  
 373 average velocity of liquid at the nozzle exit.

374 **3.3 Numerical schemes**

375 The behavior of different interpolation schemes is presented in Figure 9, Figure 10, and Figure 11

376 The order of the temporal integration schemes for phase-fraction and governing conservation equations

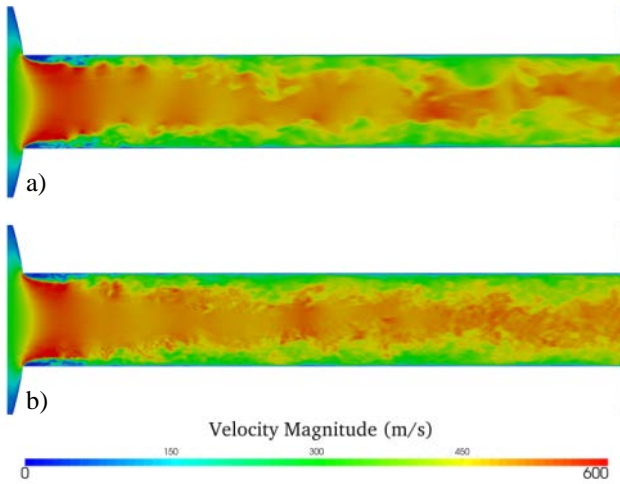
377 plays a significant role in prediction of small-scale eddies inside the nozzle orifice. As depicted in Figure

378 9, at the quasi-steady stage, employing the second-order scheme named *Backward* results in smaller scale

379 eddies in comparison to the first-order, *Euler*, approach due to higher dissipation in the first-order

380 scheme. This influences irregularities which are mainly generated by the reduction of the cross-sectional

381 area at the nozzle inlet where there is strong change in flow direction, and vena contracta phenomena  
382 [50].

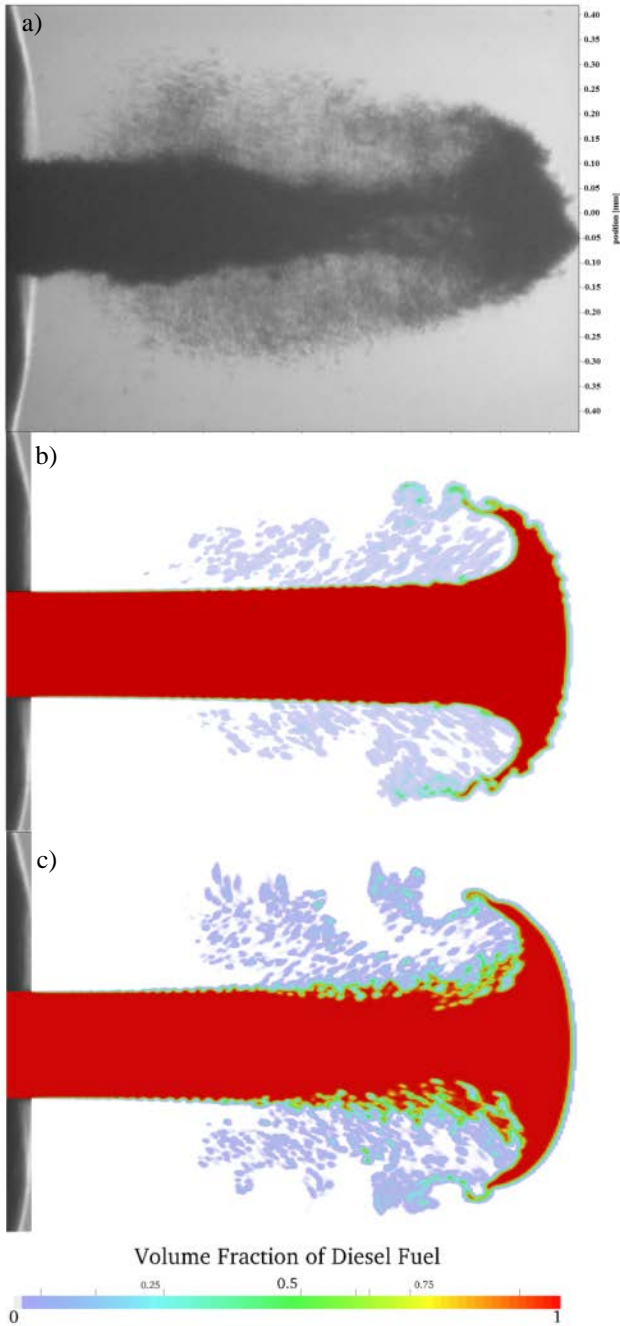


383

384 **Figure 9.** Influence of the time derivative order on prediction of turbulent structures within the nozzle  
385 orifice at quasi-steady stage ( $P_{\text{inlet}} = 1200$  bar), colored by velocity magnitude, for the fine grid case with;  
386 a) Euler, first-order and b) Backward, second-order.

387 The first-order discrete equations are more diffusive than the second-order discrete equations  
388 [41]. The impact of the time interpolation method is also seen in Figure 10, at  $14 \mu\text{s}$  ASOP. The  
389 disintegration of droplets from the liquid jet surface behind the leading edge diminishes with the first-  
390 order scheme compared with the second-order scheme. The second-order accurate interpolation scheme  
391 enables modelling of smaller fluctuations of velocity in the liquid-gas interface. Therefore, the K-H  
392 waves intensify behind the umbrella-shaped leading edge resulting in higher rates of separation. This  
393 separation narrows the liquid jet, demonstrating the necking phenomena of the spray. This necking  
394 process is weakened in the first-order interpolation scheme due to higher dissipation (in-efficiency in  
395 resolving smaller eddies) in this method. This is why the second-order scheme for time derivatives has  
396 been employed for the present study.





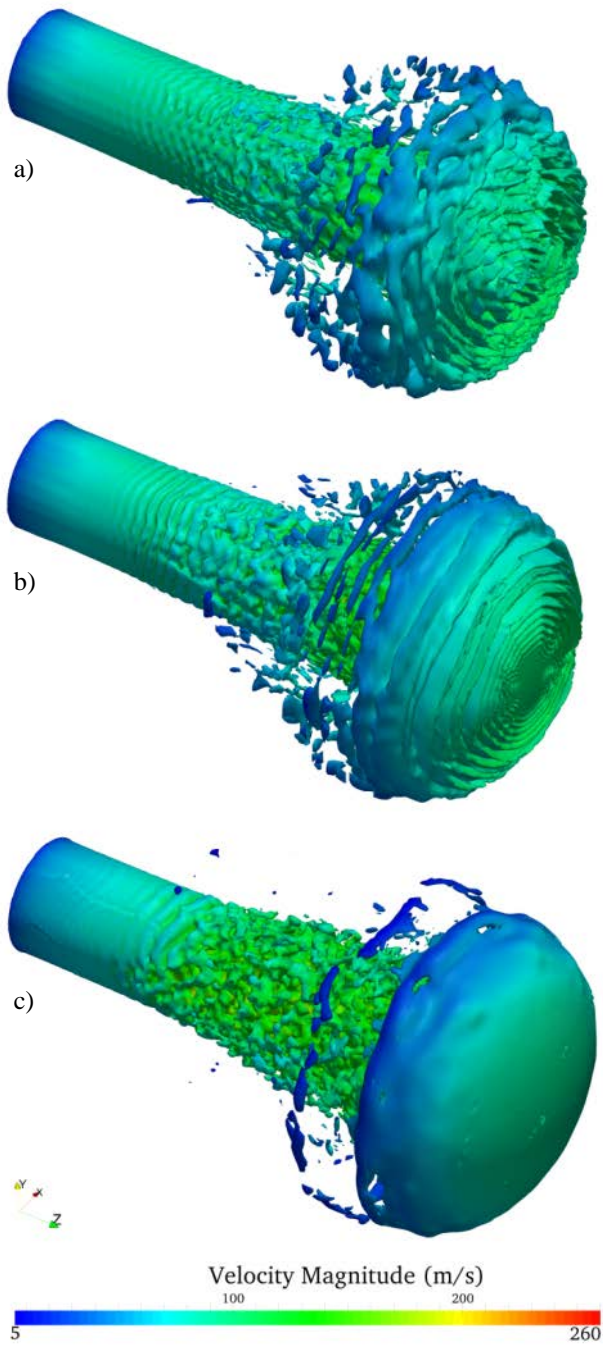
397

398 **Figure 10.** Comparison of an experimental image with numerical results showing the effect of the order  
 399 of temporal integration scheme on the jet disintegration process at  $t = 14 \mu\text{s}$  ASOP, colored by volume  
 400 fraction of diesel fuel, for the fine resolution case; a) Experiment, b) First-order, and c) Second-order.

401 The influence of the convection-specific interpolation scheme on capturing the liquid-gas interface is  
 402 illustrated qualitatively in **Figure 11** for medium grid resolution. Different ranges of first/second order  
 403 bounded numerical schemes have been investigated from the more dissipative, Total Variation  
 404 Diminishing (TVD), up to the more conservative NV schemes. The NV Gamma scheme showed a

405 smooth leading edge surface which is in agreement with DNS results of [14, 34] at a similar penetration  
406 velocity. Thus, the NV Gamma scheme has been selected for solving the convection terms. The presence  
407 of air in the liquid could play a role in the generation of surface roughness in the leading edge of the  
408 experimental jet which is not seen in the simulations.

409       Secondary interfacial instabilities known as Rayleigh-Taylor (R-T) instabilities may develop when  
410 the propagation velocity is sufficient to exceed a critical value. If R-T instability develops, it presents as a  
411 rapid crosswise modulation on the leading edge followed by shedding of drops [11]. These interfacial  
412 instabilities grow as the jet proceeds downstream and increase gas penetration into the core liquid. The  
413 latter forms ‘blobs’ joined by thin core ligaments. These blobs finally snap and complete the core breakup  
414 process. The simulations capture an umbrella-shaped leading edge which qualitatively is in agreement  
415 with the experimental results as shown in Figure 6 and Figure 7, although no spanwise instabilities due to  
416 the R-T mechanism are apparent with the NV Gamma scheme. Figure 11 demonstrates that certain  
417 convection interpolation schemes may give apparent or Rayleigh-Taylor (R-T)-like instabilities which are  
418 not necessarily physical.



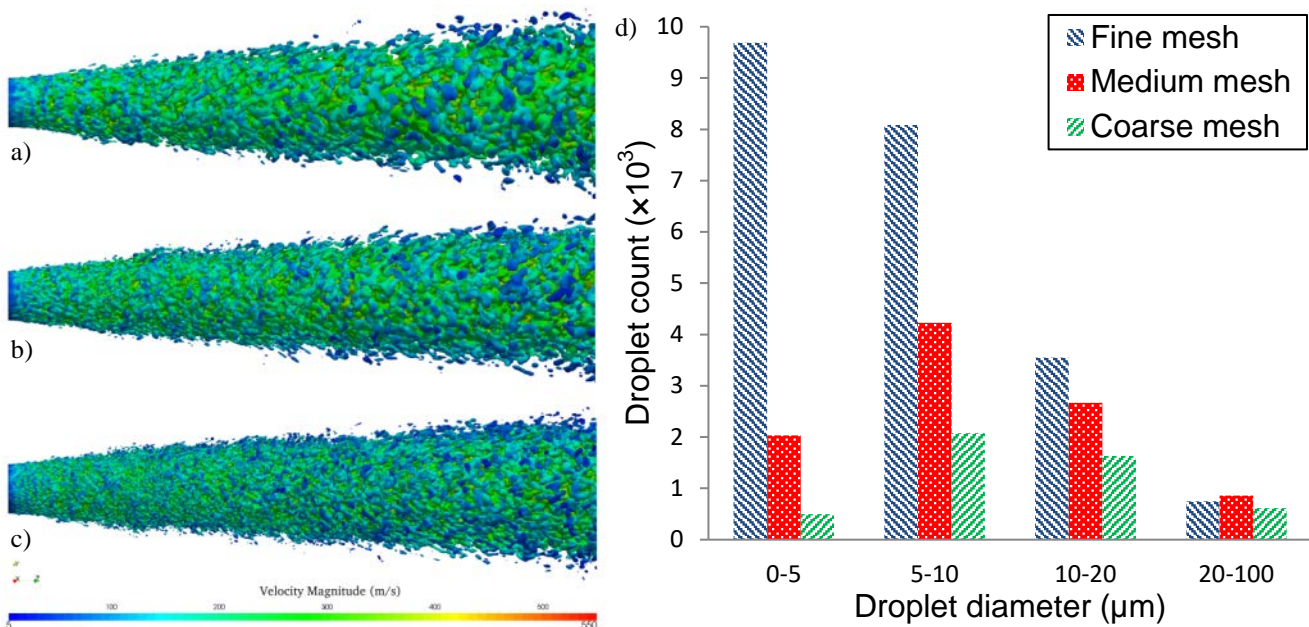
419

420 **Figure 11.** The effect of convection-specific interpolation schemes on capturing surface instabilities of  
 421 the jet beyond the nozzle exit for the medium resolution grid at  $t = 14 \mu\text{s}$  ASOP, indicated by volume  
 422 fraction of  $\gamma = 0.5$ , and colored by velocity magnitude; a) TVD, FilteredLinear, b) TVD, LimitedLinear,  
 423 and c) NV, Gamma

### 424 3.4 Spray structure of diesel fuel at quasi-steady operating condition (pressure = 1200 bar)

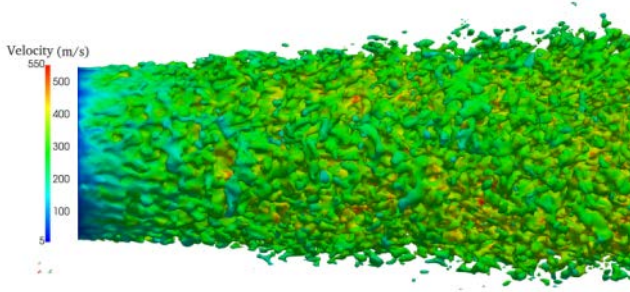
425 The atomized liquid fraction on the spray surface for the three mesh resolutions is illustrated in  
 426 Figure 12 by  $\gamma = 0.1$  isosurfaces, coloured by the velocity magnitude at the quasi-steady stage where

427 diesel fuel pressure at sac inlet is 1200 bar. The onset of primary atomization can be seen close to the  
 428 nozzle exit for the three mesh resolutions. Very fine droplets are captured near the nozzle exit noticeably  
 429 in the finest case (20 million cells) which agrees with the experimental images. The surface velocity  
 430 decelerates rapidly close to the orifice exit due to relaxation of the velocity profile. The number of  
 431 discrete droplets captured for the coarse, medium and fine meshes at the quasi-steady stage are 4830,  
 432 9494, and 22076 respectively. The increase in apparent atomization from finer meshes is due to better  
 433 prediction of the smaller-scale in-nozzle turbulent structures as presented in Figure 4, resulting in smaller-  
 434 scale surface eddies which intensify the breakup process. Consequently, the breakup rate increases in  
 435 cases with higher mesh resolution. The atomization rate at the quasi steady stage is 0.0139, 0.0148, and  
 436 0.0158 kg/s for coarse, medium and fine mesh, respectively. The finer the mesh, the finer the resolved  
 437 droplets. Mesh independence is not demonstrated due to limited computer resources and unfeasible  
 438 computation time.



439  
 440 **Figure 12.** Spray morphology within 12 nozzle diameters of the nozzle exit, indicated by isosurface of  
 441 volume fraction  $\gamma = 0.1$ , colored by velocity magnitude at quasi-steady stage ( $P_{inlet} = 1200$  bar); a) Coarse,  
 442 b) Medium and c) Fine case showing decreasing scale of surface features with increasing mesh resolution.  
 443 Panel d) shows quantitatively the greater number of fine droplets generated with finer meshes.

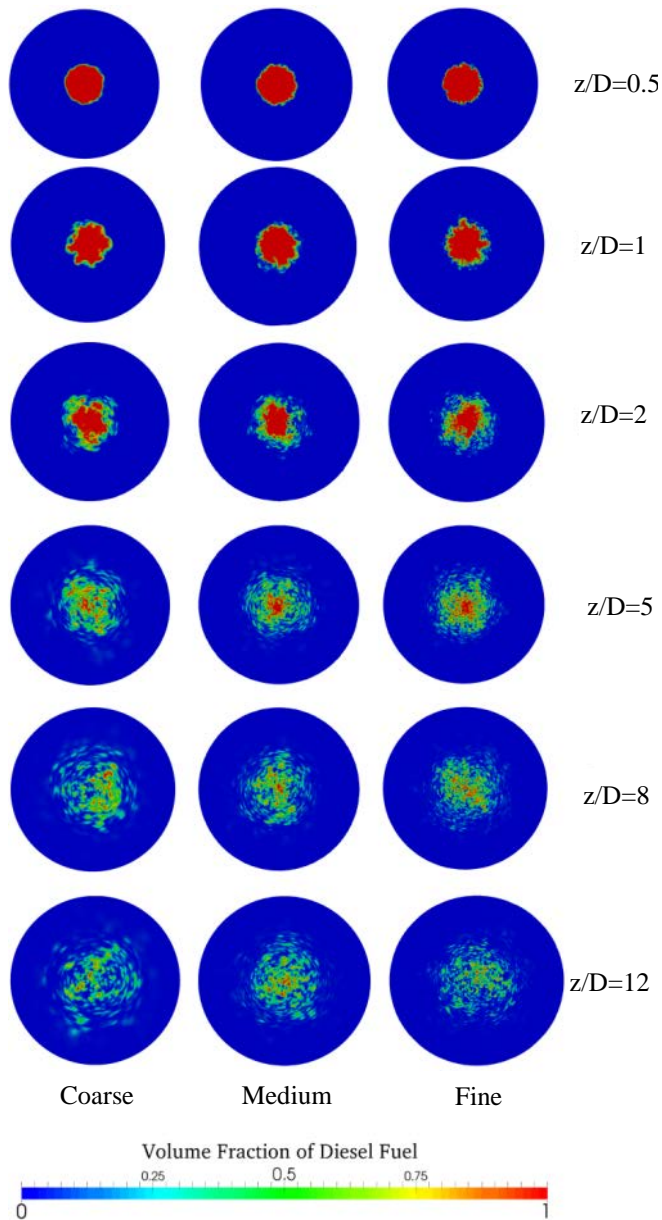
444 Figure 13 illustrates a close-up view of the jet disintegration, visualized using the isosurface of  
445  $\gamma = 0.5$  for the fine mesh case, at the quasi-steady stage. This picture represents the jet surface detachment  
446 and droplet generation, occurring even at one nozzle diameter downstream.



447

448 **Figure 13.** Close-up view showing the onset of surface breakup visualized by isosurface of  $\gamma = 0.5$   
449 colored by velocity for the fine mesh case at quasi-steady stage ( $P_{\text{inlet}} = 1200$  bar).

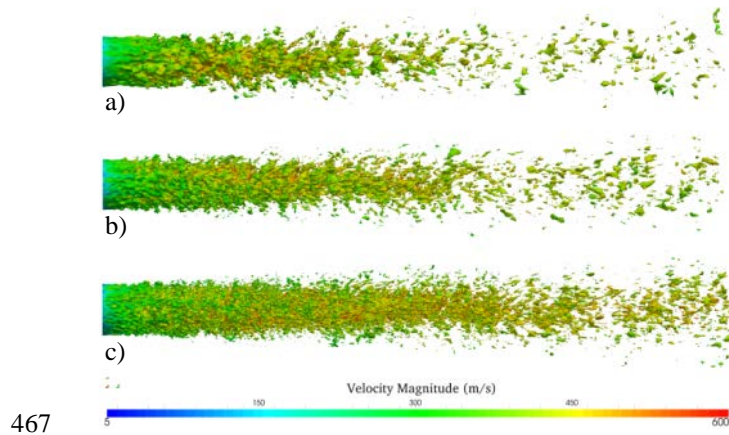
450 The growth of non-axisymmetric disintegration at different cross-sections from the nozzle exit is  
451 presented in Figure 14. The formation of small longitudinal waves can be seen at one nozzle diameter  
452 downstream of the nozzle exit. At one diameter downstream primary breakup is triggered and intensifies  
453 farther downstream. Up to 5 diameters from nozzle exit, the core breakup process is fully developed since  
454 the liquid core is narrowing to tapered ligaments. The liquid core is totally disintegrated at 8 diameters  
455 downstream, resulting in higher numbers of droplets than at the positions upstream.



**Figure 14.** Liquid distribution in cross-sectional planes at different streamwise positions downstream of the nozzle exit for the coarse (left column), medium (middle column) and fine (right column) cases at quasi-steady stage ( $P_{\text{inlet}} = 1200$  bar). The value of  $z/D$  indicates the number of nozzle diameters downstream of the nozzle exit.

Figure 15 illustrates the liquid core visualized using the  $\gamma = 0.95$  isosurface at quasi-steady stage ( $P_{\text{inlet}} = 1200$  bar) for different meshes. It can be seen that longitudinal surface perturbations develop near the nozzle exit. The liquid core tapers progressively before disintegrating into large clusters which is in accordance with the limited available data by [51]. The fine mesh case shows an extended liquid core

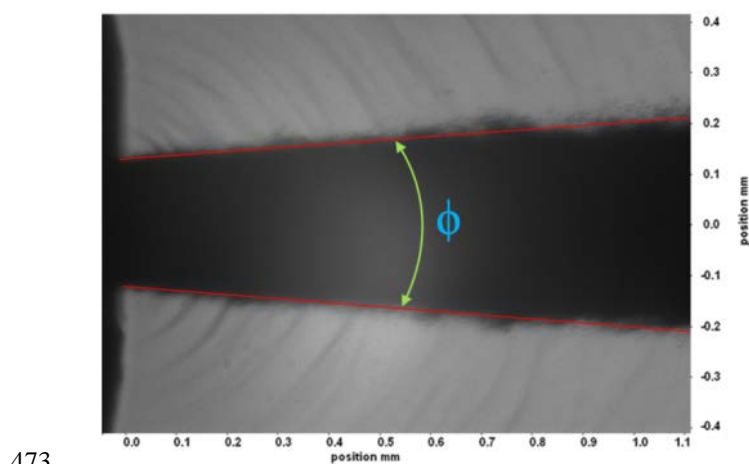
465 compared to the coarser cases. This is due to pinching-off of smaller droplets from thinner ligaments  
466 detached from the liquid jet surface which slows down the liquid core disintegration process [8, 48, 49].



467

468 **Figure 15.** Effect of mesh resolution on jet liquid core length depicted by  $\gamma = 0.95$  isosurface for  
469 a) Coarse, b) Medium and c) Fine mesh cases at quasi-steady stage ( $P_{inlet} = 1200$  bar).

470 Figure 16 depicts the early spray angle ( $\phi$ ) at quasi-steady stage, measured on a spray image using  
471 edge detection based on a threshold filter. The formation and development of shear layer instabilities can  
472 be clearly seen. The nozzle tip is apparent on the left side of the image.

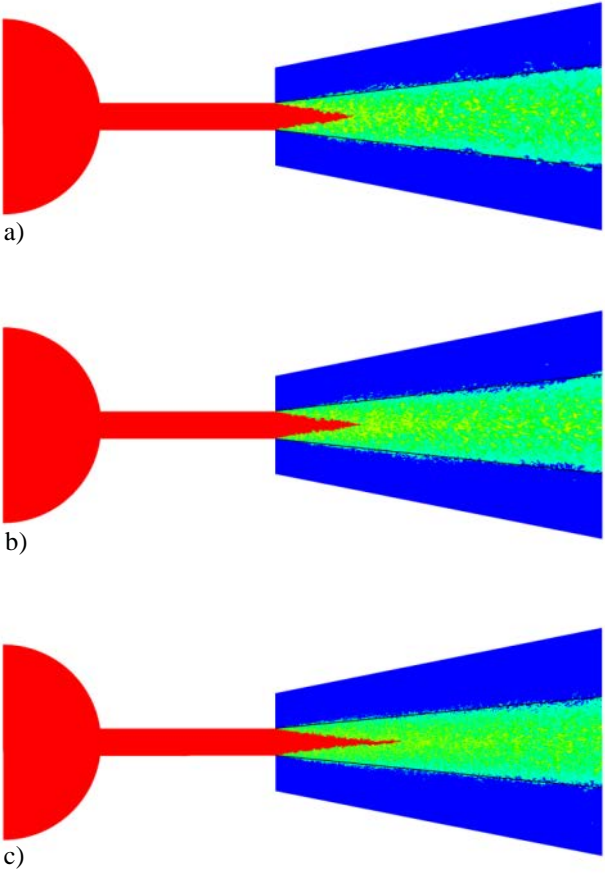


473

474 **Figure 16.** Shadowgraphy of the diesel nozzle spray at quasi-steady stage ( $P_{inlet} = 1200$  bar), using long  
475 distance microscope[45].

476 To compare the predicted numerical early spray angle with experiment, Leboissetier & Zaleski [52]  
477 core analysis was conducted. Based on this method, three different zones in the numerical data were

478 distinguished at every time step during the quasi-steady stage. The results of this analysis for three  
 479 different cases are depicted in Figure 17, showing the time-averaged structure of the atomization region.  
 480 The red zone contains only liquid (never contains gas), thus representing the liquid core; the blue region  
 481 is gas only while the green region contains sporadic liquid and gas volumes depicting the atomization  
 482 zone. The early spray angle was extracted using the outer boundary of the two phase mixture (green)  
 483 zone.



484  
 485 **Figure 17.** A Leboissetier & Zaleski [52] core analysis for, a) Coarse, b) Medium, and c) Fine at quasi-  
 486 steady stage,  $P_{inlet}=1200$  bar; red and blue region experienced only liquid and gas, respectively. The green  
 487 zone is the atomization region.

488 A summary of this investigation, gathered using these plots (Figure 17) is tabulated in Table 4,  
 489 showing the reduction in spray angle and increase in liquid core length for the higher mesh resolution  
 490 cases. For comparison, the core length predicted by Hiroyasu and Arai's correlation [17] is also shown.



491 The predicted core length appears to be too small and this may be partly due to the methods used to  
492 determine core length and partly due to the absence of a cavitation model, and thus overly high jet  
493 turbulence.

494 **Table 4.** Comparison of spray angle and liquid core length

Case	Early Spray Angle	Core Length (mm)
Experiment	$8.7 \pm 0.4^\circ$	-
Coarse	$13.22 \pm 1^\circ$	$0.71 \pm 0.05$
Medium	$12.52 \pm 0.8^\circ$	$0.73 \pm 0.05$
Fine	$11.26 \pm 0.5^\circ$	$1.151 \pm 0.02$
Hiroyasu & Arai [17]		9.13

#### 495 **4. Conclusions**

496 The general structure of primary atomization of diesel sprays was successfully characterized  
497 numerically employing an Eulerian/LES/VOF approach to capture free surfaces. The umbrella-shaped  
498 leading edge of the emerging jet was captured successfully near the nozzle exit. The experimental  
499 shadowgraphy images showed a rougher surface, greater transparency, more oblique angle and earlier  
500 disintegration of the leading edge in comparison with the numerical prediction. This is presumed due to  
501 in-nozzle air inclusions left from the previous injection event. The necking of the liquid jet behind the  
502 umbrella-shaped leading edge is captured in both experimental and numerical results. The temporal  
503 variation of jet penetration velocity and Reynolds number show favorable agreement between numerical  
504 and experimental results. The second-order temporal integration scheme and NV Gamma convection-  
505 specific interpolation scheme resulted in a better prediction of small scale eddies and jet surface structures  
506 compared with the first-order integration scheme and TVD convection-specific interpolation schemes.

507 A mesh resolution study for the two stages of the spray, initial penetration and quasi-steady, revealed  
508 that:

- 509 • fragmentation of the jet commenced close to nozzle exit (within about one diameter from exit) for  
510 the finest mesh
- 511 • modelling of the primary breakup process is enhanced with higher mesh resolution
- 512 • droplet sizes decrease with increasing mesh resolution
- 513 • smaller eddies were captured with decreasing cell size inside the nozzle
- 514 • increasing mesh resolution leads to decrease in the early spray angle and increase in the liquid  
515 core length, leading to better agreement between experiment and numerical predictions.

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