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Mesh resolution effects on DNS-VOF of primary atomization

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Abstract

In this work, we use Direct Numerical Simulation (DNS) through a Volume of Fluid (VOF) solver with Adaptive Mesh Refinement (AMR) to analyze the atomization of a pulsating round liquid jet with a narrow length scale range configuration. We propose three grid sizes based on characteristic scales we estimate from the deformation and fragmentation processes of this problem. We compute drop statistics and general spray features for each case. We found that mesh resolution affects the atomization rate and the probability density function of droplets size and position, not only for the under-resolved drops but all liquid structures. The two simulations with higher grid refinement presented volume-weighted distribution with minor differences. Therefore, we propose assessing the accuracy of atomization simulations based on the volume fraction of under-resolved structures.

Keywords: Atomization, Volume of Fluid (VOF), Adaptive Mesh Refinement (AMR), Basilisk

1. Introduction

Primary atomization is a complex phenomenon of great interest because, as described by [1], it is present in several natural processes (e. g. sea-waves, waterfalls) and technical applications (e. g. internal combustion engines, spray coating, spray drying, disease propagation).

Atomization is a multiscale phenomenon whose characteristic length scales depend mainly on the turbulent intensity and the acting interface forces. As [2] discussed in their paper, this is one of the features that make it difficult to apply Direct Numerical Simulations (DNS) to study primary atomization problems. In particular, high-speed injection of round liquid jets presents atomization at high Reynolds and Weber numbers which produce a wide range of flow length-scales. This feature increases the computational cost of DNS, as discussed by [3], and also makes it more difficult to study the problem experimentally, as noted by [4].

Nevertheless, the growth of computational power and the optimization of numerical methods during the first two decades of the 21st century have driven some research on this topic. Some of the goals from these works are improving the understanding of fragmentation mechanisms, especially in the dense spray region, and developing low-cost models with direct technological applications, such as injector nozzle design. In the following paragraph, we summarize some research projects that illustrate the current state of the art on primary atomization DNS.

On one of the first fuel injection DNS analysis, [5] simulated a diesel jet at moderate speeds, applying advanced interface representation techniques (CLSVOF) and a turbulent boundary condition based on the works of [6]. From these results, [3] estimated the effect of momentum transport phenomena at the sub-grid scales and proposed algebraic interface models in the context of an ELSA (*Eulerian-Lagrangian Spray Atomization*), developed and validated by [7] and [8] among others.

A few years later, [9] studied different atomization regimes with moderate Reynolds and Weber numbers using a second-order level-set method. In their analysis, they describe in detail the jet tip deformation and fragmentation process and how they interact with the vortex dynamics. Although the boundary conditions used in these analyses do not accurately represent the internal flow of a fuel injector, these simulations capture in great detail the growth of hydrodynamic instabilities on the surface of the jet. Recently, [10] proposed atomization models using DNS results to develop a Sub-Grid Scale

38 (SGS) breakup model, based on ligament pinch-off, to perform Large Eddy
39 Simulations (LES) of diesel combustion.

40 In the particular case of fuel injection, validation through experimental
41 data is still a big challenge. Even if there are benchmark injection exper-
42 iments, such as the *spray A* developed by the [11], they measure only the
43 disperse spray zone during periods of a few milliseconds. In contrast, [12]
44 studied the *spray A* case in a low-velocity regime using the Volume of Fluid
45 (VOF) method on uniform cartesian meshes. They reproduced the first 20 μs
46 of injection, reaching the breakup length and the early development stages
47 of the dense spray.

48 Regarding more fundamental studies, [13] and [14] analyzed the deforma-
49 tion of cylindrical jets for a broad spectrum of flow regimes. They describe
50 the vortex dynamics and how it affects the instabilities developed along with
51 the jet core, analyzing the interaction between turbulence and fragmenta-
52 tion mechanisms. Using similar methods [15] described the breakup process
53 on planar jets and how the fragmentation modes develop for a different set
54 of parameters. Even if these analyses characterize the growth of interface
55 instabilities in detail, they do not give further insights on how this process
56 impacts on the final drop size distribution.

57 Besides these difficulties, DNS is still used to study early atomization
58 stages on fuel injection problems. [16] and [17, 18] applied the VOF technique
59 with Adaptive Mesh Refinement (AMR) to analyze the primary atomization
60 of diesel, biodiesel, and gasoline on injection problems at moderate speeds.
61 Through a complete statistical characterization of the cases, these works
62 describe the overall evolution of the fuel spray. These simulations employed
63 the *Basilisk* C library, by [19]; we obtained the results presented in this
64 manuscript using an updated version of these numerical tools.

65 In this work, we employ the *Basilisk* VOF-AMR solver to analyze the
66 primary atomization of a pulsating liquid jet, using different grid sizes based
67 on the characteristic length scales of the flow. Section 2 describes the mathe-
68 matical model and numerical techniques implemented on the Basilisk solver.
69 Section 3 defines the atomization problem designed for this study and the
70 criteria employed on the grid convergence analysis. Section 4 describes the
71 general features of the injection process and presents the drops statistics,
72 comparing the results for the three refinement levels. Finally, section 5 sum-
73 marizes the conclusions and gives some insight regarding future works.

74 The main goal of the present analysis is to find quantitative descriptions
75 for low grid resolution effects on primary atomization DNS. The following

76 questions serve as a guide for that objective:

- 77 • Is it possible to determine *a priori* the grid resolution needed to repro-
78 duce the physical behavior of primary atomization?
- 79 • Is it possible to assess the numerical accuracy of a simulation without
80 running a mesh convergence analysis?
- 81 • What should be the threshold to determine which liquid structures are
82 resolved or not? How to measure the impact of the under-resolved
83 drops?
- 84 • How does poor mesh resolution affect the global properties of a spray,
85 such as the atomized volume or the interface area density?

86 2. Mathematical model and numerical method

87 The Momentum-Conserving VOF (MCVOF) solver described in this sec-
88 tion is based on the compressible solver by [20], considering incompressible
89 flow. These schemes are described in detail by [21] and, more recently, by
90 [18]. The three articles aforementioned present validation cases to test the
91 consistency and robustness of the momentum-conserving advection schemes
92 and the discrete balance of surface tension forces. In particular, [18] also
93 report numerical results for the spray G benchmark case. The general layout
94 of the model and numerical methods are given next.

95 2.1. Incompressible Multiphase Flow model

96 The mass and momentum conservation equations for incompressible and
97 isothermal flow can be expressed as:

$$\nabla \cdot \vec{u} = 0 \tag{1}$$

$$\frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot (\rho \vec{u} \vec{u}) = -\nabla p + \nabla \cdot (2\mu \mathbf{D}) + f_\sigma \tag{2}$$

99 where $\vec{u}(\vec{x}, t)$ is the velocity field and $p(\vec{x}, t)$ is the pressure field. Tensor \mathbf{D} is
100 defined as $\frac{1}{2} [\nabla \vec{u} + (\nabla \vec{u})^T]$. The properties of the flow (ρ and μ) are density
101 and viscosity. The last term on the right-hand side on the Navier-Stokes
102 Equation 2 represents the surface tension force:

$$f_\sigma = \sigma \kappa \vec{n}_s \delta_s \tag{3}$$

103 where the surface tension coefficient σ is considered constant. The force only
 104 acts at the free surface, hence the Dirac function δ_s , and also depends on the
 105 interface shape, particularly on its curvature κ and normal \vec{n}_s .

106 In the context of the one-fluid formulation for multiphase flows, the color
 107 function $c(\vec{x}, t)$ gives the phase spatial distribution on the domain, taking
 108 value $c(\vec{x}_p, t) = 1$ if the point p is filled with one phase and $c = 0$ otherwise.
 109 The interface is then located in the discontinuity surface of the c function,
 110 defining δ_s , \vec{n}_s , and κ . The color function transport is given by the following
 111 Equation:

$$\frac{\partial c}{\partial t} + \nabla \cdot (c\vec{u}) = c \nabla \cdot (\vec{u}). \quad (4)$$

112 where the right-hand side is equal to zero due to Equation (1).

113 2.2. Numerical method

114 The numerical implementation used in this work represents the free-
 115 surface using the Piecewise Linear Interface Capturing (PLIC) VOF method
 116 by [22] and [23]. In the Finite Volume Method (FVM) context, the mean
 117 value of the c function on a cell is:

$$f_\Omega = \frac{1}{\Delta\Omega} \int_\Omega c(x, t) dV, \quad (5)$$

118 where $\Delta\Omega$ is the volume of the cell Ω . Then f_Ω is the volume fraction of the
 119 main phase ($c = 1$) in the cell. The mixture properties on the cell can then
 120 be computed by arithmetic means:

$$\rho_\Omega = f\rho_l + (1 - f)\rho_g \quad \mu_\Omega = f\mu_l + (1 - f)\mu_g \quad (6)$$

121 From this point on, we drop the cell-based subscript for the sake of clarity.
 122 The following equations are valid on each cell and must be solved for all of
 123 them. In this context, the approximate projection method by [24] is used to
 124 solve coupling between Equations (1) and (2), considering that the velocity
 125 (\vec{u}) is staggered in time VOF (f) and pressure (p), which is noted next by the
 126 superscript indicating the time-step for each variable. The discrete equations
 127 can then be expressed as in [25]:

$$\frac{f^{n+\frac{1}{2}} - f^{n-\frac{1}{2}}}{\Delta t} + \nabla \cdot (\vec{u}_n f_n) = c_c \nabla \cdot \vec{u}_n \quad (7)$$

128

$$\frac{\rho \vec{u}^* - \rho \vec{u}^n}{\Delta t} + \nabla \cdot (\rho^{n+\frac{1}{2}} \vec{u}^n \vec{u}^n) = \nabla \cdot [\mu^{n+\frac{1}{2}} (\mathbf{D}^n + \mathbf{D}^*)] + (\sigma \kappa \delta_s \vec{n}_s)^{n+\frac{1}{2}} \quad (8)$$

129

$$\nabla \cdot \left(\frac{\Delta t}{\rho^{n+\frac{1}{2}}} \nabla p^{n+\frac{1}{2}} \right) = \nabla \cdot \vec{u}^* \quad (9)$$

130

$$\vec{u}^{n+1} = \vec{u}^* - \frac{\Delta t}{\rho^{n+\frac{1}{2}}} \nabla p^{n+\frac{1}{2}} \quad (10)$$

131

132

133

134

Here c_c is the contraction function used in the split volume fraction advection scheme from [26], $c_c = 1$ if $f > 0.5$ and $c_c = 0$ otherwise. The advection terms in Equations (7) and (8) involve VOF and momentum fluxes respectively. In this context:

$$\nabla \cdot (\vec{u}_n f_n) = \frac{\sum_{f,i} F_{f,i}}{\Delta \Omega} \quad F_{f,i} = f_a (\vec{u}_{f,i} \vec{S}_f), \quad (11)$$

135

$$\nabla \cdot (\rho^{n+\frac{1}{2}} \vec{u}^n \vec{u}^n) = \frac{\sum_{f,i} F_{f,i}^{\rho \vec{u}}}{\Delta \Omega} \quad F_{f,i}^{\rho \vec{u}} = [(\rho_l \vec{u})_f f_a + (\rho_g \vec{u})_f (1 - f_a)] (\vec{u}_{f,i} \vec{S}_f), \quad (12)$$

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where $F_{f,i}$ and $F_{f,i}^{\rho \vec{u}}$ are the VOF and momentum fluxes through the face i , computed from the face fraction $f_a = V_a / (u_{f,i} S_f)$ represented in Figure 1: the left side shows a cell where the light gray region is the main phase volume and the dark gray region is the main phase volume transported to the neighbor cell. The face-reconstruction of the velocity, \vec{u}_f , and momentum for each phase, $(\rho_l \vec{u})_f$ and $(\rho_g \vec{u})_f$, are computed by the second-order upwind BCG scheme, by [27], using a minmod slope limiter. The right side of Figure 1 shows that the VOF function f implicitly defines the momentum fields that must be advected following Equation 12 to ensure consistency between mass and momentum transport.

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We use the semi-implicit Crank-Nicholson scheme to compute the diffusive flux due to the viscous term in Equation (8). We discretize the surface tension force term at the face with the same scheme employed to compute the pressure gradient. This ensures a well-balanced formulation that reduces spurious currents, as explained by [28]. The interface curvature is computed using second-order stencils based on height functions computed by an analytical formulation from [29]. Equations (9) and (10) are the projection steps that will ensure mass conservation for the velocity field at the step $(n + 1)$. The solver procedure is as follows: **MCVOF method** Given the fields at a time-step n : $f^{n-1/2}$, u^n :

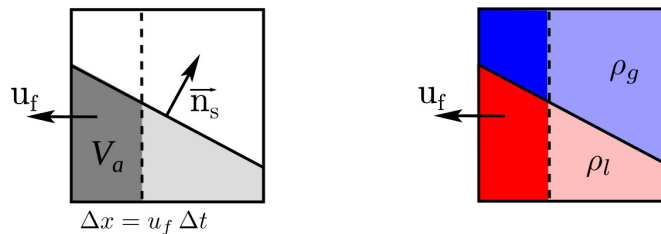


Figure 1: Flux computation example, considering a single square cell. *Left*: VOF flux computation on the left face, where normal velocity is u_f , of a cell with interface normal \vec{n}_s . *Right*: schematics on how the density field affects momentum transport.

- 156 1. Compute face fluxes from equations (11) and (12)
- 157
- 158 2. Integrate VOF function by Equation (7) to get $f^{n+1/2}$
- 159
- 160 3. Integrate the momentum Equation (8), adding the advection fluxes and
- 161 the right hand-side terms, to get the velocity approximation \vec{u}^*
- 162
- 163 4. Solve Equation (9) to compute pressure $p^{n+1/2}$
- 164
- 165 5. Correct \vec{u}^* by Equation (10) to compute the next step velocity \vec{u}^{n+1}
- 166

167 In the simulations reported, we applied Adaptive Mesh Refinement (AMR)
 168 in the octree grid Basilisk implementation. In this context, the whole domain
 169 is the root cell, with refinement level 0 and side L_0 ; adding a refinement level
 170 to a cell consist of dividing it into eight children with a grid size equal to half
 171 the size of its parent. Given the maximum refinement level (\mathfrak{L}), the small-
 172 est grid size $\Delta = L_0/2^{\mathfrak{L}}$. The refinement criterion is based on bounding a
 173 wavelet-based error estimation. Further details on this technique theoretical
 174 basis can be found in the works by [30], [31], and [32].

175 3. Simulation setup

176 We analyze the atomization of a circular jet injected on a gas-filled cubical
 177 chamber. This problem is solved using AMR with three grid refinement levels
 178 and the same refinement criteria. The physical properties of each phase

179 are based on low-velocity diesel injection, following [5], using a pulsating
 180 boundary condition for the inlet, as done by [16, 17]. This configuration
 181 has a narrow length-scale range and a simple deterministic injection velocity
 182 profile independent of grid refinement.

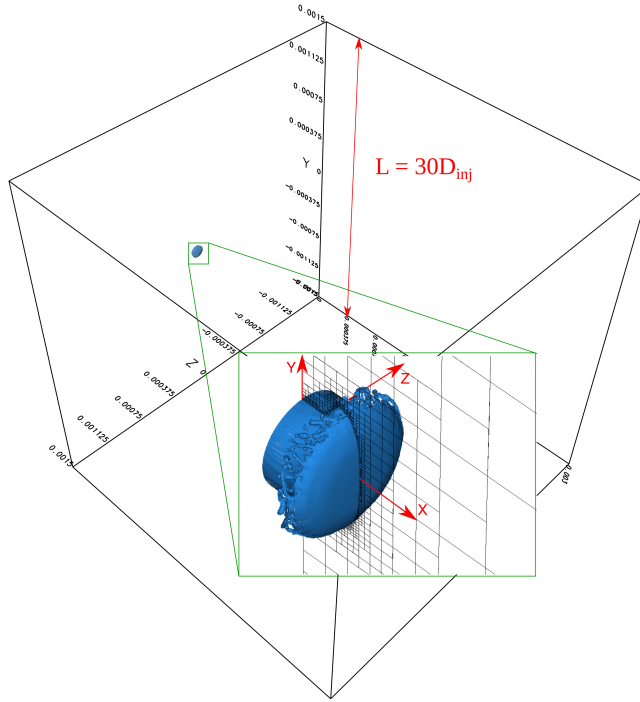


Figure 2: Isometric view:domain and detail of initial evolution ($t = 0.2 \mu s$) with adaptive refinement

183 The same adaptive refinement criteria are applied in all the simulations.
 184 We bound the *wavelets* error estimates of the volume fraction f and the ve-
 185 locity field \vec{u} , defining as maximum thresholds for the local error estimations
 186 $E(f) < 10^{-5}$ and $E(\vec{u}) < 1$ m/s respectively.

187 3.1. Problem definition and boundary conditions

188 The jet of diameter D_{inj} is injected in a cube with a length of $30 D_{inj}$,
 189 as represented in Figure 2. The boundary condition on the injection face
 190 ($x = 0$) imposes the no-slip condition everywhere except on the liquid section

191 $(\sqrt{y^2 + z^2} < D_{inj}/2)$ where the injection velocity is:

$$u_x(t) = U_{inj} [1 + \zeta \sin(f 2\pi t)] \quad f = \text{St} \frac{U_{inj}}{D_{inj}}. \quad (13)$$

192 This periodic perturbation has been employed in the works of [16] to ac-
 193 celerate the atomization process near the nozzle. Moreover, this deterministic
 194 boundary condition produces simple hydrodynamic instabilities that are well
 195 resolved for all the grid size employed. It is worth to mention that [13, 14]
 196 reproduced early spray formation dynamics on simulations of axisymmetric
 197 jets with a single frequency perturbation, showing that this level of sim-
 198 plification still preserves the behavior of the problem of interest. All the
 199 simulations were performed using the same boundary condition with $\zeta = 0.1$
 200 and $\text{St} = 1.3$. On the remaining cube sides, we allow free outflow: $\partial_n \vec{u}_\Gamma = 0$
 201 and $p_\Gamma = 0$.

202 We use the phase properties of an academic diesel injection problem,
 203 following the work [5], summarized in Table 1. This configuration presents
 204 a relatively small ratio between macro and micro length-scales, reducing the
 cost of resolving all the relevant scales for atomization phenomena.

Table 1: Physical properties of the system

| $D_{inj}[\mu\text{m}]$ | $U_{inj}[\text{m/s}]$ | $\rho_g[\text{kg/m}^3]$ | $\rho_l[\text{kg/m}^3]$ | $\mu_g[\text{kg}/(\text{m s})]$ | $\mu_l[\text{kg}/(\text{m s})]$ | $\sigma[\text{N/m}]$ |
|------------------------|-----------------------|-------------------------|-------------------------|---------------------------------|---------------------------------|----------------------|
| 100 | 100 | 25 | 696 | 10^{-5} | 1.2×10^{-3} | 0.06 |

205 In this context, the present mesh convergence study considers three maxi-
 206 mum refinement levels, named M1, M2, and M3. The mesh step for each case
 207 will be defined by the end of the next section, based on the flow characteristic
 208 length scales.
 209

210 3.2. Dimensionless groups and characteristic scales

211 The dimensionless groups relevant to a round liquid jet atomization prob-
 212 lem are:

$$\text{We}_l = \frac{\rho_l U_{inj}^2 D_{inj}}{\sigma} \quad \text{Re}_l = \frac{\rho_l U_{inj} D_{inj}}{\mu_l} \quad \rho^* = \frac{\rho_l}{\rho_g} \quad \mu^* = \frac{\mu_l}{\mu_g} \quad (14)$$

213 where ρ_l and ρ_g are the densities of each phase, in this case, liquid and gas
 214 respectively. The viscosity coefficients are noted by μ_l and μ_g . σ is the
 215 surface tension coefficient, U_{inj} is the injection mean velocity and D_{inj} is
 216 the nozzle diameter. The Reynolds and Weber numbers can be computed
 217 for both phases. They also can be used to express the Ohnesorge number
 218 ($Oh_l = \sqrt{We_l}/Re_l$). In order to verify the accuracy of the incompressibility
 219 hypothesis, the Mach number ($Ma_g = U_{inj}/\sqrt{kRT}$) should be lower than 0.3.
 220 The characteristic time based on the problem kinematics is $t_c = (D_{inj}/U_{inj})$,
 221 which in this case is exactly equal to $1 \mu s$.

Table 2: Dimensionless description of the case

| ρ^* | μ^* | Re_l | Re_g | We_l | We_g | Oh_l | Ma_g |
|----------|---------|--------|--------|--------|--------|--------|--------|
| 27.8 | 83.3 | 5800 | 25000 | 11600 | 430 | 0.0186 | 0.175 |

222 We analyze several characteristic lengths, described in detail in Appendix
 223 .1, to define the grid resolutions for our simulations. We summarize the values
 224 of these length scales (\boldsymbol{l}) on Table 3. We briefly describe the relevance of each
 225 length-scale next.

226 The Kolmogorov scales in each phase (η_g and η_l) define the requirements
 227 for resolving all the turbulent structures: according to [33], resolving all scales
 228 by pure DNS is only possible if $\Delta < 2\eta$. The Hinze scale (ζ) represents the
 229 biggest drop that does not suffer breakup by turbulent effects, as described
 230 by [34].

231 Given the effects of the shear stresses on the jet surface, Kelvin-Helmholtz
 232 Instability (KHI) dominates the deformation stage. Therefore, we consider
 233 the critical wavelength for KHI, λ_c^{KH} , based on linear stability theory con-
 234 sidering a simplified shear flow on the jet surface. This is a conservative
 235 reference for the smallest unstable interface perturbations.

236 Finally, we consider [35] estimations of the relevant length scales for sheets
 237 and ligaments breakup: λ_s and D_{lig} . The short wavelength λ_s is reported by
 238 these authors to be independent of the jet geometry, as it is also discussed
 239 by [36] who use a similar estimation for round jets. Regarding the diameter
 240 D_{lig} , we use the same mass conservation relation to estimate the size of
 241 ligament detached from the sheet developed from the jet tip, measuring the
 242 film thickness locally on previous simulations.

243 It is important to recall that all these estimations are conservative, based
 244 on simplified geometries and flow conditions, aiming to consider the most
 challenging scenarios.

Table 3: Characteristic length scales.

| l | η_g | η_l | ζ | λ_c^{KH} | λ_s | D_{lig} |
|-----------|----------|----------|---------|------------------|-------------|-----------|
| $[\mu m]$ | 0.078 | 0.131 | 9.71 | 1.56 | 3.01 | 2.69 |

245 Based on these length scales, we choose the mesh step for simulation M1
 246 to be $\Delta_1 = 1.46\mu m$ corresponding to a maximum octree-refinement level of
 247 11. M2 and M3 will use level 12 and 13 respectively, resulting in $\Delta_2 = 0.73\mu m$
 248 and $\Delta_3 = 0.37\mu m$.

250 In this context, the M1 simulation will not be able to resolve short-
 251 wavelength unstable hydrodynamic instabilities. M2 will barely represent
 252 λ_c^{KH} with two cells and M3 will even capture stable interface perturbation.

253 Regarding fragmentation, the M1 grid resolution will not be able to rep-
 254 resent ligaments predicted by [35] formulation, as of $\Delta_1 > 0.5D_{lig}$. The M2
 255 resolution will be able to reproduce ligaments with $D > 0.54D_{lig}$ and M3
 256 with $D > 0.26D_{lig}$.

257 We run the cases M1 and M2 until they reached 25 μs of physical time.
 258 These simulations required approximately 3 500 and 50 000 CPU-hours re-
 259 spectively. At $t = 25\mu s$, mesh M1 had 87 237 340 cells and mesh M2 had
 260 414 813 435 cells. We run the M3 simulation until $t = 11.2\mu s$, which took
 261 218 000 CPU-hours and finished with 602 257 783 cells. We performed all the
 262 simulations on the machine *Irene* administrated by TGCC.

263 4. Results and discussion

264 In this section, we describe the physical problem and the fragmentation
 265 mechanism and we compare statistics for the three simulations to analyze
 266 the grid resolution effects. We first define the parameters to characterize
 267 the spray and individual droplets. The Sauter Mean Diameter (SMD) of a
 268 spray is defined as:

$$SMD = 6 \frac{\sum_i^N V_i}{\sum_i^N A_i} \quad (15)$$

269 where V_d and A_d are the volume and area of the "d" droplet respectively.
 270 N is the total amount of drops in the spray. The SMD is equivalent to the
 271 diameter of a spherical drop with the same surface area density than the
 272 whole spray; smaller SMD imply higher area to volume ratio.

273 For single droplets, diameter and shape will be measured in terms of
 274 equivalent volume diameter (D_{30}) and sphericity (ψ) which can be defined
 275 as:

$$D_{30} = \left(6 \frac{V_d}{\pi}\right)^{(1/3)} \quad D_{32} = 6 \frac{V_d}{A_d} \quad \psi = \frac{D_{32}}{D_{30}} \quad (16)$$

276 It should be noticed that D_{32} is equivalent to the SMD of a single drop, and
 277 it is always smaller than D_{30} ; except in spherical shapes, for which $\psi = 1$.

278 4.1. General overview

279 Figure 3 shows a side view of the interface at regular time intervals of
 280 $5 \mu s$ for the M2 simulation, at subfigures (a-d), and the evolution of some
 281 spray parameters for the three simulations.

282 The snapshots in the figure let us grasp the general aspects of the core
 283 deformation and atomization. The frames (a) and (b) show that the tip de-
 284 formation requires more than $5 \mu s$ to produce the first liquid sheets. Between
 285 5 and $10 \mu s$, the first group of drops and short ligaments detaches from the
 286 tip. This ring of liquid structures expands radially and moves on the axial
 287 direction much slower than the rest of the jet, as can be seen in frames (c) and
 288 (d). Between 15 and $20 \mu s$ a second, denser, group has formed. It is worth to
 289 notice that at this time, the drops in the first ring are almost spherical.

290 The graphs in subfigures (e) and (f) show the evolution of the ratio be-
 291 tween droplet volume ($V_{drops}(t) = \sum_i^N V_i$) and injected volume ($V_{inj}(t) = \int_t Q(\tau) d\tau$).
 292 The linear scale graph, subfigure (e), shows that at the beginning of injection
 293 ($t < 5 \mu s$) the total atomized volume is less than 1%. Between $5 \mu s$ and $10 \mu s$
 294 the atomization rate increases significantly and at $t = 20 \mu s$, around 10% of
 295 the injected volume is atomized. The graph with the logarithmic scale, sub-
 296 figure (f), allows us to observe the evolution of the volume fraction in drops
 297 smaller than $3 \mu m$. After $t = 10 \mu s$, they represent less than 0.5% of the total
 298 injected volume for the three cases.

299 The last graph of Figure 3, subfigure (g), represents the spray SMD. Be-
 300 fore $5 \mu s$ the amount of drops is so small that each new liquid structure affects
 301 the SMD significantly; it is also worth noticing that, as seen in subfigure (f),
 302 mostly small drops are produced. The slope of the SMD graph changes sig-
 303 nificantly near $8 \mu s$. At the same instant, the atomization rate increases, as

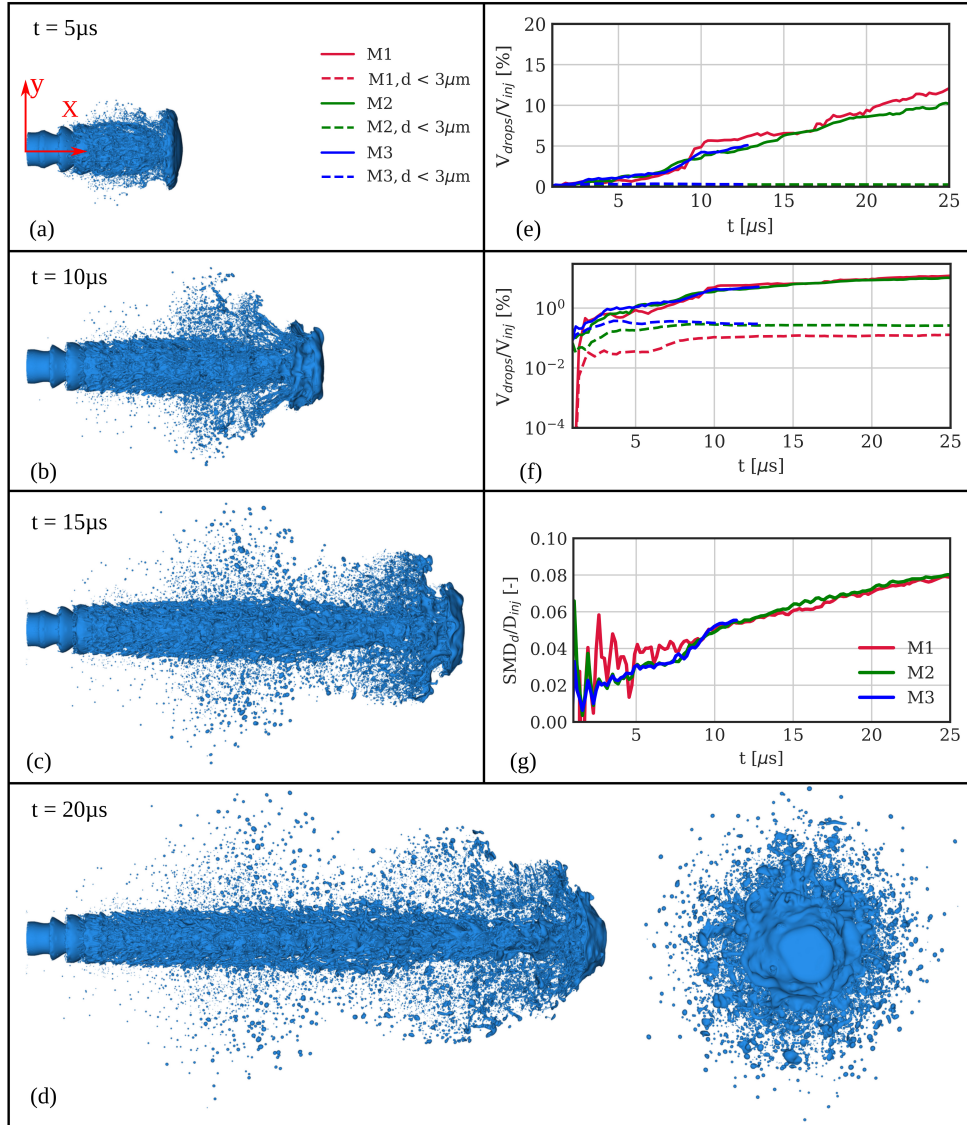


Figure 3: Side view of M2 simulation (a-d). Temporal evolution of drop volume fraction in linear (e) and logarithmic (f) scales, to compare the total atomized volume and the volume of the small drops respectively. Evolution of the spray Sauter Mean Diameter (SMD) for the three mesh resolutions (g).

304 seen in subfigure (e). This change can only be possible due to the production

305 of large drops, given that the small drops fraction remains almost constant,
 306 as can be noted in subfigure (f).

307 These three graphs show that small drops are produced from early stages
 308 of atomization, in contrast to large drops and ligaments that need more
 309 time to develop from shear-induced instabilities. Regarding grid resolution
 310 effects, we see that M1 presents a higher atomization rate, subfigure (e), and
 311 a lower volume fraction of small drops, subfigure (f). Remarkably, M1 and
 312 M2 present good agreement on the spray SMD after $t = 10 \mu s$, despite the
 313 aforementioned differences.

314 Figure 4 compares the evolution of the core's D_{32} and spray SMD for
 315 the three simulations. M2 and M3 present good agreement (less than 2%
 316 difference) for both drops and core behavior, even at early atomization stages.
 317 It is worth noticing that, despite this agreement, the liquid core of M1 has
 318 a much lower D_{32} and, therefore, a higher surface density. From this result,
 319 we can claim that the M1 generates drops and surface area faster than the
 finer simulations.

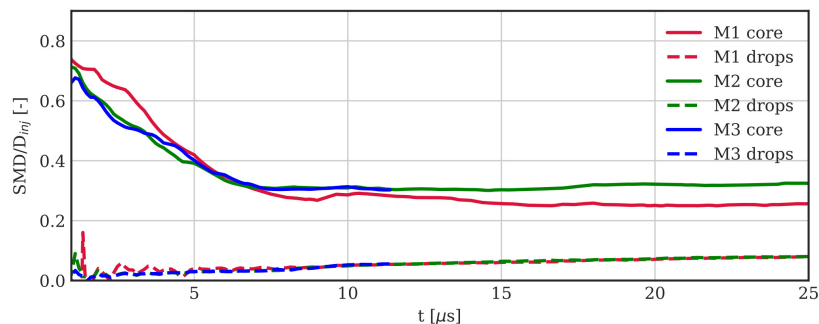


Figure 4: Core and drops Sauter Mean Diameter (SMD) for the three mesh resolutions.

320

321 A better understanding of the relation between the jet evolution analyzed
 322 in the frames (a-d) in Figure 3 and the grid resolution effect on the spray
 323 characteristics requires a more detailed observation of the breakup mech-
 324 anisms. These processes have been studied by [9] and [16], among others.
 325 From this starting point, we highlight some aspects of the fragmentation pro-
 326 cess in Figure 5 to study how grid resolution can affect them. In this figure,
 327 the black circle marks the formation of holes in a region of a liquid sheet
 328 with velocities between 0 and 75m/s, denoting the presence of shear-induced
 329 instabilities.

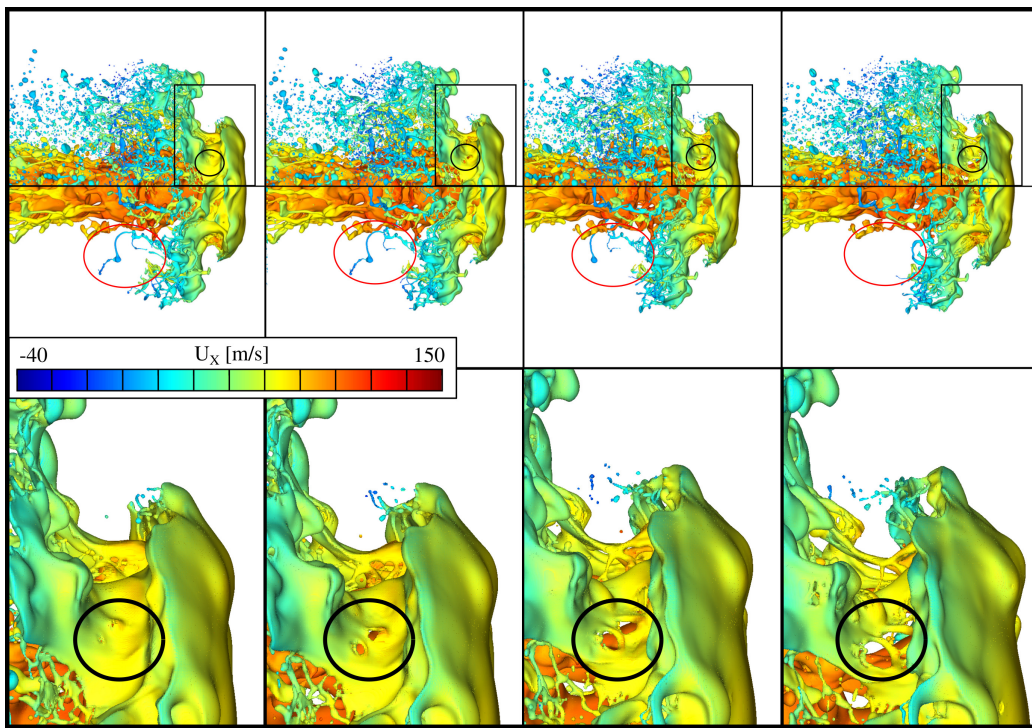


Figure 5: M2 simulation: side view of the jet at $t = (14.4, 14.6, 14.8, 15.0)\mu s$, colored by axial velocity (u_x). The top row shows the jet's core and detached drops, where a hole formation and expansion process is highlighted with a circle. The middle row shows the evolution of the jet core, filtering the drops out; the oval here highlights the detachment of two ligaments due to capillary effects. The bottom row shows a zoomed image of the head region highlighted by a rectangle in the top row, showing the hole dynamics with more detail.

330 On the other hand, the detached filament marked by the red ellipse is
 331 practically at rest but its diameter is considerably reduced; the high aspect
 332 ratio and deformation resulting from aerodynamic effects will produce non-
 333 linear capillary breakup, even if the shear stresses are not enough to induce
 334 fragmentation.

335 The previous analysis is also valid for the rest of the jet. The growth of
 336 instabilities in all the jet surface can be seen in Figure 6, where the liquid
 337 fraction on the middle plane is represented in black. This figure shows that
 338 perturbations in the rest of the jet surface produce thin structures as well.
 339 We can also observe in this frame the loss of mass near the axis. Even if

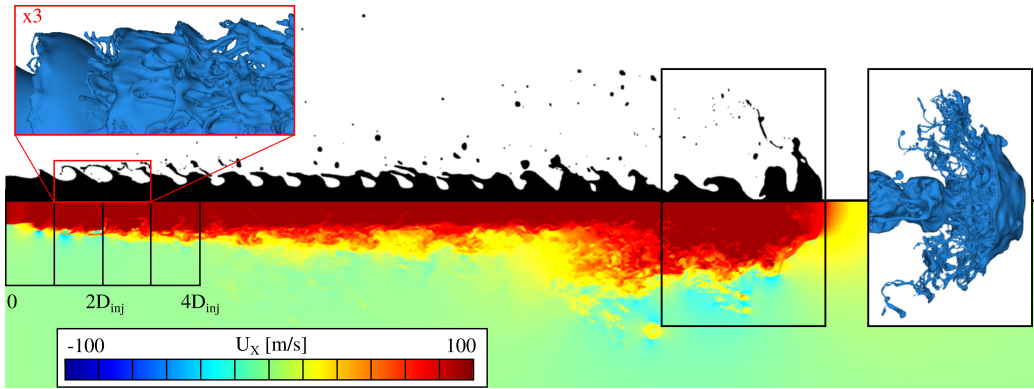


Figure 6: f (top) and u_x (bottom) fields at plane $z = 0\mu\text{m}$ for $t = 20\mu\text{s}$ of M2 simulation. The box on the top-left corner contains an isometric zoomed view detail of the near nozzle region. The box on the right shows an isometric view of the jet head.

340 connectivity between the tip and the core has almost been lost along the
 341 axis, the tip has not yet detached from the liquid core, as it is shown in the
 342 detail of the core tip to the right.

343 Figure 6 also shows the growth of the long-wavelength perturbation in
 344 the near nozzle region ($x \in [0, 2D_{inj}]$), where shear stresses induce a Kelvin
 345 Helmholtz Instability (KHI) on the axis direction. The KHI growth rapidly
 346 generates thin liquid sheets that suffer fragmentation before reaching $x =$
 347 $3D_{inj}$, as we show in the red box detail; after this point, the instability has
 348 lost its axial symmetry due to the turbulent behavior of the mixing layer.
 349 These dynamics follow the generation of transverse instabilities described
 350 by [13] and [14]. As the holes expand, they form ligaments and drops that
 351 detach from the core and impact on the upwind instabilities on the jet surface,
 352 increasing its fragmentation rate.

353 In this context, regarding grid resolution effects on the fragmentation pro-
 354 cess, it is worth to remark that both the sheet perforation and the ligament
 355 pinch-off occur when two different interfaces meet in the same cell; from that
 356 instant on, the grid cannot resolve the coherent structure. This fact could
 357 explain why coarse grids present faster fragmentation and, therefore, higher
 358 atomization rate.

359 Another spray feature that might be affected by poor mesh resolution is
 360 the spatial distribution of the drops, partially described in Figure 7.

361 The left column shows the complete jet for each simulation, colored by

362 axial velocity (U_x) and the right column shows a two-way histogram where
 363 each pixel color represents the volume fraction of the drops aligned with the
 364 ray parallel to the axis and located at that particular (Y, Z) position.

365 The side views show several effects on the drop positions. First, in finer
 366 grids more drops are generated in the near nozzle region. Another effect
 367 of mesh refinement is the radial expansion of the spray: the M3 simulation
 368 presents the furthest drops. In the three cases, the drops detached from
 369 the jet tip are almost still, which means that they will not travel downward
 370 significantly. We can also notice that the M1 simulation has larger liquid
 371 structures near the jet tip; most of them present a high degree of deformation.
 372 This fact will be addressed quantitatively in the next section.

373 The scatter histograms show that, as we use higher refinement levels,
 374 mass distribution around the axis gets more even and covers a larger radius.
 375 Increasing mesh resolution also increases the entrainment rate of drops in
 376 the mixing layer: the cases M2 and M3 present drops almost $R_{inj}/2$.

377 4.2. Effects of mesh-resolution on drop statistics

378 In this section, we analyze the mesh resolution effects on drop size and
 379 shape. We first compare the droplets D_{30} distributions for the times $t =$
 380 $[6, 9, 11] \mu s$ in Figure 8 and then focus on the spray at the latter time, fitting
 381 the distributions in Figure 9.

382 At all times, the most frequent diameter is 2Δ ; smaller diameters cannot
 383 be resolved, hence their presence is minimal. For example, M3 presents
 384 almost 10.000 drops in the range $D_{30} \in [0.5 : 1] \mu m$ while M2 produces less
 385 than 1000 drops in the same range. These graphs also show that big droplets
 386 ($D_{30} > 12 \mu m$) take longer periods of time to develop, as there are almost
 387 no droplets in that range at $6 \mu s$, but all the simulations show more than 10
 388 drops bigger than $10 \mu m$ at $t = 11 \mu s$.

389 The histograms can be compared quantitatively by, for example, fitting
 390 them using a log-normal distribution,

$$N(d) = \frac{C}{d} \exp \left[-\frac{(\ln d - \hat{\mu})^2}{2 \hat{\sigma}^2} \right]. \quad (17)$$

391 Figure 9 shows the fitted histogram (weighted by D_{30}) using a logarithmic
 392 scale on both axes. This representation has been used by [37] to ease the
 393 comparison between distributions. We also report the mean ($\hat{\mu}$) and standard
 394 deviation ($\hat{\sigma}$) in this Figure. It is worth to notice that the mean value for the

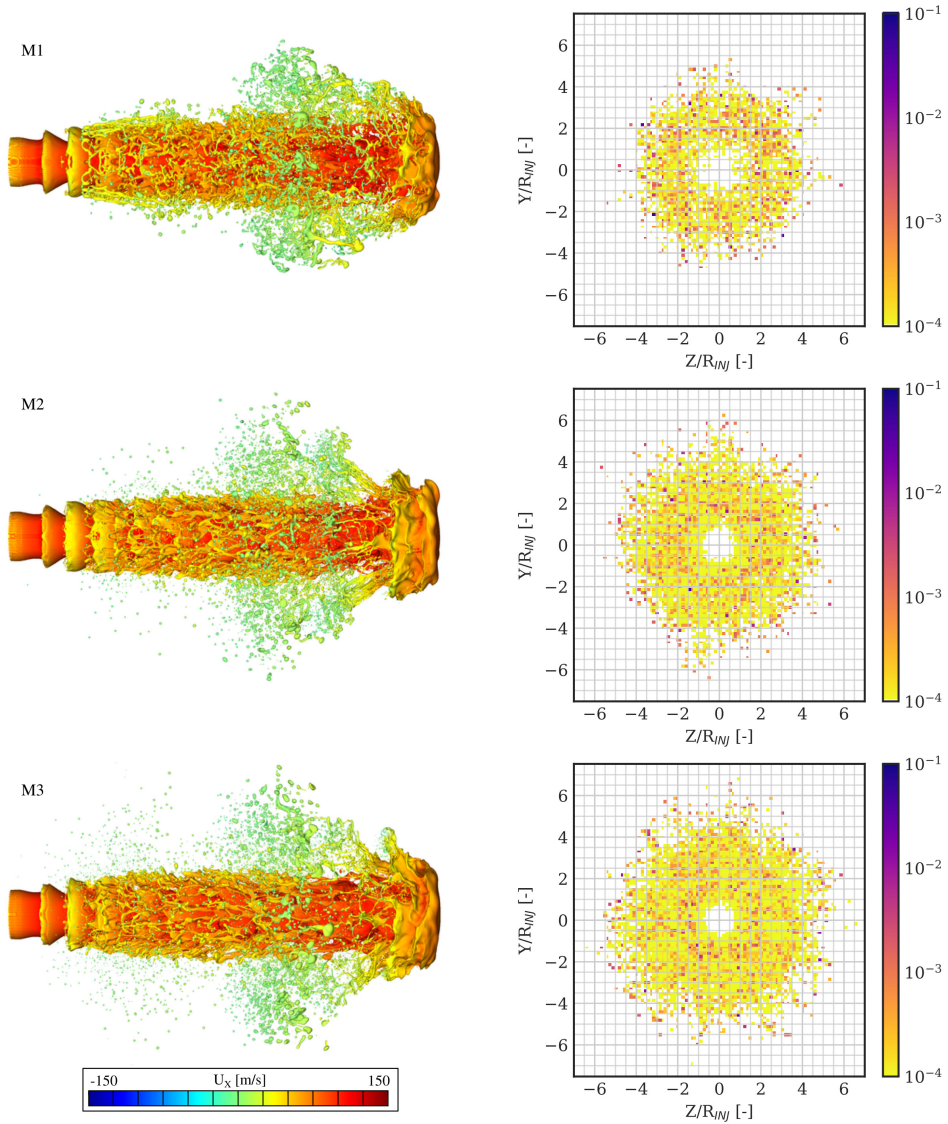


Figure 7: Mesh convergence: side view colored by velocity (left) and scatter histograms showing radial mass distribution on drops (right) for $t = 11 \mu s$. Simulations M1 (top), M2 (middle) and M3 (bottom).

395 M1 simulation is of the same order that the grid size, while M3 could resolve
 396 its mean diameter with almost three cells.

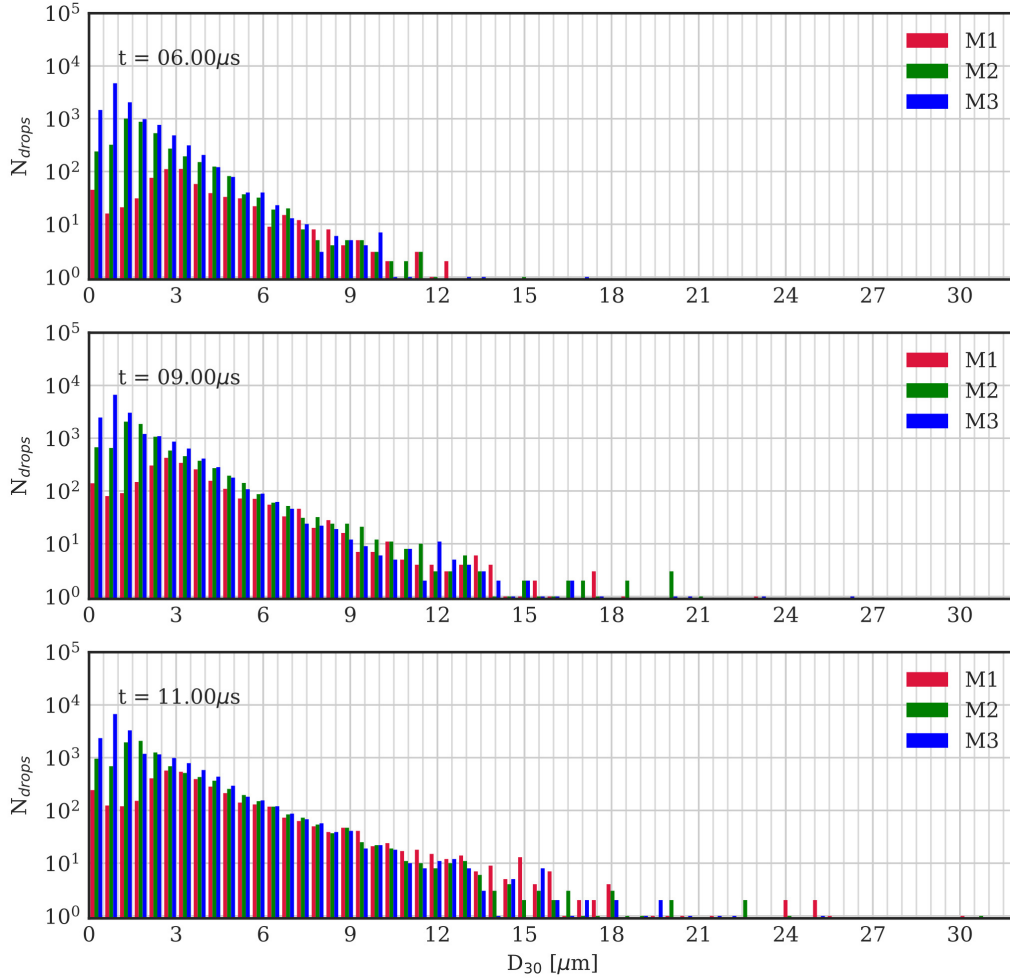


Figure 8: Drop size (D_{30}) histograms for the three simulations (M1, M2, M3) at three different times $t = (6, 9, 11) \mu s$. Bin width is $0.5 \mu m$.

397 If we now consider the volume-weighted PDF in Figure 10, the volume
 398 fraction of the small droplets is negligible: drops with $\Delta D_{30} < 2 \mu m$ represent
 399 less than 2% of the atomized volume. Moreover, even if there are just a few
 400 large liquid structures, which will eventually break up, these are much more
 401 significant in terms of volume fraction. For longer simulation times, the
 402 number of large drops will be higher, and the effect of small droplets will be
 403 less significant. These facts explain why the SMD in Figure 3 are considerably

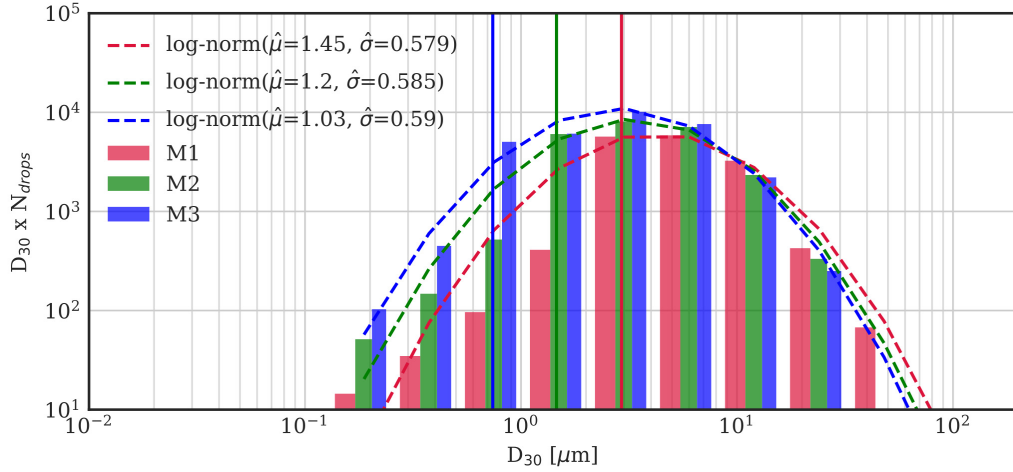


Figure 9: Log-normal PDF fitting for range $[1-30]\mu\text{m}$. Vertical lines at $D_{30} = 2\Delta$. Bin widths based on power of 2, starting from $[0.125-0.25]\mu\text{m}$

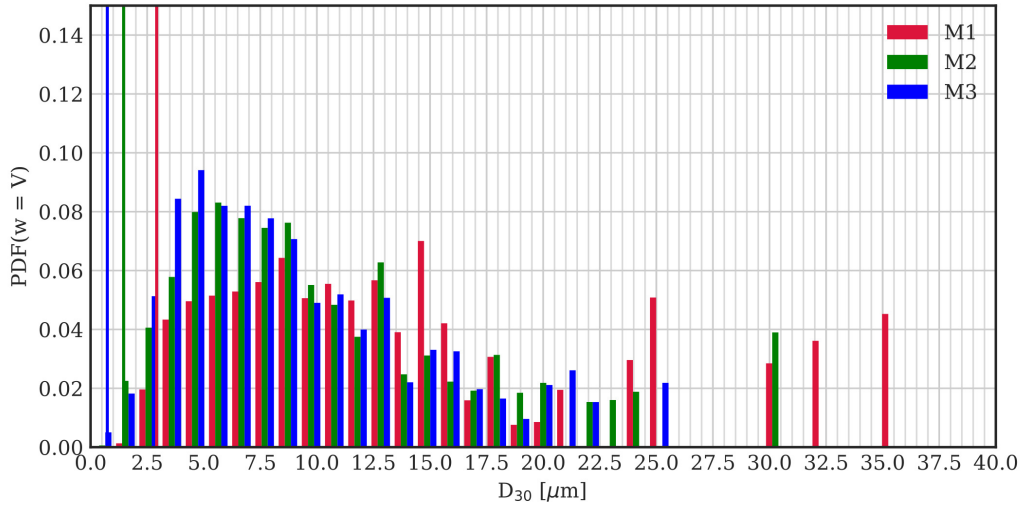


Figure 10: Volume weighted PDF at $t = 11\mu\text{s}$. Vertical lines at $D_{30} = 2\Delta$. Bin width is $1\mu\text{m}$

404 different before $t = 5\mu\text{s}$, where large drops have not formed yet, but tend to
 405 similar values after the first ligaments detach from the jet tip.

406 Figure 11 presents the Cumulative Density Function (CDF) scaled by the
atomized liquid fraction.

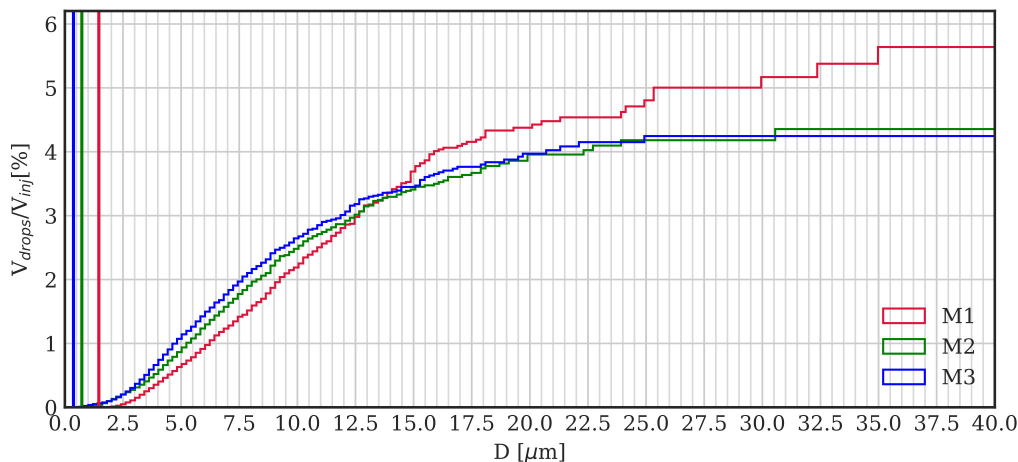


Figure 11: Cumulative distribution weighted by volume at $t = 11 \mu s$. Vertical lines placed at $D_{30} = 2\Delta$.

407
408 This graph shows that, at $t = 11 \mu s$, the M1 simulation predicts that the
409 atomized liquid volume will be 30% higher than the one predicted by the
410 other simulations (about 4.5% of the injected volume), which is consistent
411 with the (e) and (g) graphs in Figure 3. At this instant, M2 and M3 present
412 good agreement for all the diameter ranges. Both simulations predict that
413 less than 4.5% of the injected liquid will atomize in drops.

414 Figure 12 shows the sphericity distribution normalized by the number of
415 drops and liquid volume.

416 We should recall that lower ψ values correspond to higher deformation.
417 For example, a cylinder with a 5:1 length-to-radius ratio has $\psi \approx 0.69$. This
418 structure is unstable and will eventually suffer fragmentation or turn spheri-
419 cal due to surface tension. Therefore, the number of low ψ ligaments and
420 sheets will only be significant if their production rate is equal or higher than
421 their fragmentation rate. We can see in the graph that highly deformed struc-
422 tures ($\psi \leq 0.7$) represent almost 30% of the drop count for M1 and more
423 than 70% of the atomized volume. In contrast, M2 predicts that around 31%
424 of the atomized volume will be highly deformed, much closer to the M3 pre-
425 diction of 25%. Another relevant observation on these results is that more

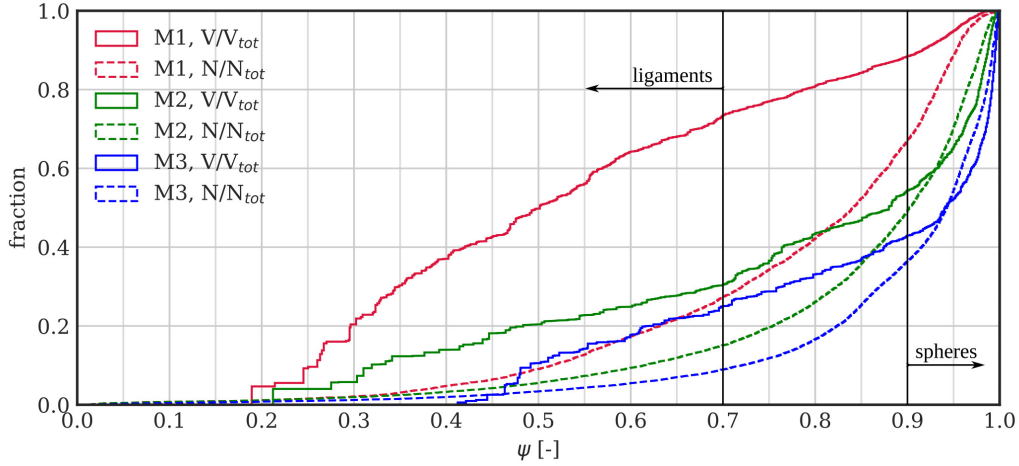


Figure 12: Sphericity distribution, weighted by drop number and atomized volume.

426 than 45%, both in volume and drop count, of the atomized liquid structures,
 427 are almost spherical ($\psi \geq 0.9$) for M2 and M3, while only 10 % of the atom-
 428 ized volume has this characteristic in M1. To summarize, coarse simulations
 429 cannot resolve the stable structures and have a higher production rate of
 430 skewed ligaments, the ψ distribution is shifted to lower values. In contrast,
 431 more than 60% of the drops on M3 present a stable shape and will probably
 432 not suffer further fragmentation.

433 All these results concern a single instant on spray development. As Figure
 434 3 shows, $t = 11\mu s$ is just by the end of the initial transient development of jet
 435 topology. To get a better comparison of the three cases during this process,
 436 Figure 13 presents the temporal evolution of the accumulated drops volume
 437 fraction grouped in ranges of $2\mu m$. In this representation, for example, we see
 438 that the M2 simulation (green) has only 15% of the liquid volume in drops
 439 with $D_{30} < 2\mu m$ at $t = 1\mu s$, and we see that this fraction decreases with
 440 time, reaching 2% at $12\mu s$. These graphs show that, for all the cases, liquid
 441 structures with $D_{30} > 20\mu m$ are formed after $8\mu s$. The M1 case presents
 442 the earliest generation of big ligaments and the highest volume fraction of
 443 large structures (e. g. drops with $D_{30} > 20\mu m$ represent 40% of the volume
 444 at $t = 9.4\mu s$).

445 Regarding small droplets, we can notice that M2 and M3 present similar
 446 behavior after $9\mu s$: the volume fraction on that range decreases slowly; in

447 both cases these fractions are approximately 2% by $t = 11\mu s$. For the M1
448 simulation, the volume fraction of drops in this range is less than 0.5% after
449 $2\mu s$.

450 Even if the size distribution is quite similar for M2 ($\Delta = 0.73\mu m$) and
451 M3 ($\Delta = 0.37\mu m$) grids, it is worth noticing that trends are not the same
452 and the breakup length has not yet been reached. Moreover, at $t = 10\mu s$
453 for example, the fraction on the range ($D_{30} > 20\mu m$) shows the biggest
454 discrepancy between M2 and M3. At the final sampling time ($t = 12\mu s$)
455 the volume fraction on the lowest range ($D_{30} < 2\mu s$) is almost negligible on
456 both M2 and M3 cases. The biggest difference between these results in the
457 ranges of $D_{30} < 10\mu m$ is 2% of the total volume. Taking the M3 result
458 as a reference, M1 underestimates the volume fraction of $D_{30} < 10\mu m$ by
459 approximately 15%.

460 5. Final remarks and future work

461 We presented Detailed Numerical Simulations of a pulsating round liq-
462 uid jet for a regime based on diesel injection at low velocities using the
463 VOF technique with AMR. Based on these results, we described the breakup
464 mechanisms and discussed how poor grid resolution accelerates fragmenta-
465 tion by merging interfaces that meet in a single cell. This effect increases the
466 atomization rate of the jet and over-predicts its surface density.

467 We then analyzed the impact that grid resolution has on the statistical
468 features of the spray generated by atomization. We found that it affects
469 not only the capability of generating small droplets but also the frequency
470 of ligament detachment. As a consequence, a simulation with coarser mesh
471 will have less small drops, more large liquid structures, and probably a higher
472 atomized volume. We found that comparing the Probability Distribution
473 Function weighted by volume highlights both issues. The cumulative PDF,
474 presented in Figure 11, is a useful tool to evaluate the atomization error due
475 to mesh resolution and its extension to Figure 13 shows the trend of this
476 error through time.

477 For the analyzed primary atomization problem, with $Re_l = 5800$ and
478 $We_l = 11600$, simulations with a grid resolution of $\Delta = D_{inj}/137$ (M2) and
479 $\Delta = D_{inj}/274$ (M3) present drop size distributions with similar volume frac-
480 tion in the small diameter range ($D_{30} < 4\mu m$), which are of order 10% by the
481 end of the initial tip development process. The agreement through all the di-
482 ameter ranges (less than 2%, as seen in Figure 13) indicates that using higher

483 refinement levels will affect a small volume fraction of the drops, mainly the
484 under-resolved structures. The prediction of shape, based on sphericity, pre-
485 sented higher discrepancies: M2 stable ($\psi > 0.7$) volume fraction was 5%
486 higher than the M3 prediction. Results from the M1 simulation differ more
487 than 40%, which impairs the capability of this simulation to predict, for ex-
488 ample, the stability of drops in the dense spray region. For the particular
489 application of designing a near nozzle fuel injection DPM, for example, the
490 small discrepancies between M2 and M3 would not make significant differ-
491 ences, but using M1 results would be unacceptable.

492 We also found that the increase of the atomization rate due to poor mesh
493 resolution affects the position of the drops: faster fragmentation of liquid
494 sheets from the jet tip reduces the radial expansion of the spray, as shown in
495 Figure 7.

496 Based on these results, we briefly discuss each of the questions at the end
497 of section 1.

498 Regarding the determination *a priori* of the grid size required to perform
499 DNS of primary atomization: we have proposed a set of length scales, de-
500 fined by the problem dimensionless groups, that give the minimal refinement
501 requirements to reproduce turbulence, deformation and breakup phenom-
502 ena. If the grid cannot resolve any of these scales, especially those related
503 to deformation and breakup, the simulation will not capture the breakup
504 mechanisms properly. Nevertheless, using grid sizes even smaller than these
505 reference lengths does not guarantee that the numerical error will be negli-
506 gible, that will also depend on the accuracy requirements.

507 Regarding the assessment of numerical accuracy without running a mesh
508 convergence analysis, we believe that a reliable parameter to quantify the
509 impact that under-resolved structures have on the overall result is the volume
510 fraction of the smallest relevant drops. This criterion would be valid for most
511 of the applications that care about areas and volumes and not on drop count
512 or minimal drop diameter.

513 The threshold to classify under-resolved structures is also an open ques-
514 tion that depends on the particular application. From a geometric perspec-
515 tive, drops with less than 2 cells per diameter cannot be represented with
516 interface capturing methods; moreover, the numerical error of VOF-PLIC
517 representation will probably be significant for drops with less than 8 cells
518 per diameter. From a practical point of view, we need that drops preserve
519 their physical behavior during processes such as deformation, fragmentation,
520 and translation. In the context of atomization, if drops with 8 cells per di-

521 ameter are present in a stable regime and if this stability is preserved in the
522 numerical results we could consider that these drops are resolved enough for
523 our purpose, even if their shape is not accurately represented.

524 Regarding how poor mesh resolution affects the global properties of the
525 simulated sprays: we found that it affects the shape and position of both
526 small and large liquid structures; hence, under-resolved simulations predict
527 denser sprays with a lower fraction of stable drops.

528 It is worth to notice that the simulated time did not reach a fully devel-
529 oped breakup length, neither produced a statistically stationary spray. One
530 of our future goals will be extending these simulations to analyze the behav-
531 ior after the jet tip detachment. Moreover, we will also study the impact
532 of turbulence on atomization. Another future use of these results is to de-
533 velop Sub-Grid Scale models to perform Large Eddy Simulations in Basilisk.
534 Afterward, we hope to simulate fuel injection cases closer to practical appli-
535 cations (e. g. spray A) and analyze how the flow regime (mainly We_l and
536 Re_l) impacts on the mesh resolution required to bound numerical breakup.

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656 **Appendices**

657 *Appendix .1. Estimation of flow characteristics scales*

658 Turbulence is one of the main features of atomization that produce multi-
659 scale behavior. As described by [38], the Kolmogorov and Hinze scales are
660 relevant on atomization. [39], based on self-similar turbulence theory, gives
661 an estimate of the length scale of viscous dissipation phenomena. Following
662 [33], this value can be estimated from the relevant macro scale (D_{inj}) and the
663 Reynolds number. [40], on the other hand, defines the maximum diameter
664 of drops that can resist pressure fluctuations without breaking up. In this
665 context,

$$\eta = \frac{D_{inj}}{\text{Re}^{3/4}} \quad \epsilon = \frac{\nu^3}{\eta^4} \quad \zeta = 0.75 \left(\frac{\sigma}{\rho_g} \right)^{3/5} \left(\frac{\epsilon}{\rho_g} \right)^{-2/5} \quad (.1)$$

666 where η is the Kolmogorov scale, ϵ is the turbulent energy dissipation rate and
667 ν is the relevant kinematic viscosity. The Hinze scale ζ is, as aforementioned,
668 a measure on the biggest droplets that can resist turbulence fluctuations. It
669 should be noted that in the problems where a mixing layer develops, the
670 average droplet size is usually considerably less than ζ , as explained by [38].

671 On the other hand, jet deformation and fragmentation mechanisms in-
672 volve the growth of hydrodynamic instabilities. On primary atomization
673 problems, the effects of tangential relative velocity to the interface, related
674 to Kelvin-Helmholtz Instability (KHI), are particularly important. In this

675 context, [41] use linear stability theory to analyze the growth of a periodic
 676 perturbation (e. g. sine function) on a planar interface separating two differ-
 677 ent fluids on layers which have a relative velocity U . They give, considering
 678 inviscid flow, the following dispersion relation:

$$\omega(k) = \left[\frac{\rho_g \rho_l (\Delta U)^2}{(\rho_g + \rho_l)^2} k^2 - \frac{\sigma}{(\rho_g + \rho_l)} k^3 \right]^{1/2} \rightarrow \lambda_c = 2\pi \frac{(\rho_g + \rho_l) \sigma}{\rho_g \rho_l (\Delta U)^2}. \quad (.2)$$

679 where ω is the wave frequency, which depends on the flow parameters and
 680 on the perturbation wave number $k = 2\pi/\lambda$. The wave will only be unstable
 681 if $\omega(k)$ has a positive imaginary component. Hence, the critical value λ_c
 682 is the minimal wavelength for which the disturbance grows and therefore the
 683 perturbations with $\lambda < \lambda_c$ will remain stable.

684 On the other hand, fragmentation mechanisms related to capillarity are
 685 also affected by shortwave instabilities, as discussed by [42, 35, 43]. As
 686 the sheets and filaments reduce their thickness and speed, the perturbations
 687 evolve as Rayleigh-Taylor (sheets) or Plateau-Rayleigh (ligaments) instabil-
 688 ities. In both cases, the *breakup* occurs by a reduction of the section until
 689 the opposite surfaces of the liquid structure come into contact. In particular,
 690 [35] approximation of the wavelength with the maximum growth rate based
 691 on linear analysis of liquid sheets on gas streams:

$$k_s = \frac{\rho_g (U)^2}{2\sigma} \rightarrow \lambda_s = \frac{4\sigma\pi}{\rho_g (U)^2}. \quad (.3)$$

692 From this length, they also estimate the diameter of the ligaments as a
 693 function of the liquid sheet initial thickness (e_0), from which they also give
 694 an approximation for the size of drops produce from ligament breakup,

$$D_{lig} = \sqrt{\frac{8e_0}{k_s}} \rightarrow D_{drop} = 1.88 D_{lig} (1 + 3 \text{Oh}_l)^{1/6}. \quad (.4)$$

695 The initial thickness of the sheet will, of course, depend on the jet ge-
 696 ometry and flow conditions. *A priori* estimations could be done based on,
 697 for example, KHI wavelength. Nevertheless, the values reported on Table 3
 698 consider e_0 as the thickness of sheets still attached to the jet core, as can be
 699 seen in Figure .14 which shows a side view of the VOF field on the middle
 700 plane. It can be noted that as the sheet moves away from the tip its thickness
 701 is reduced, forming films of less than $2 \mu\text{m}$ thick.

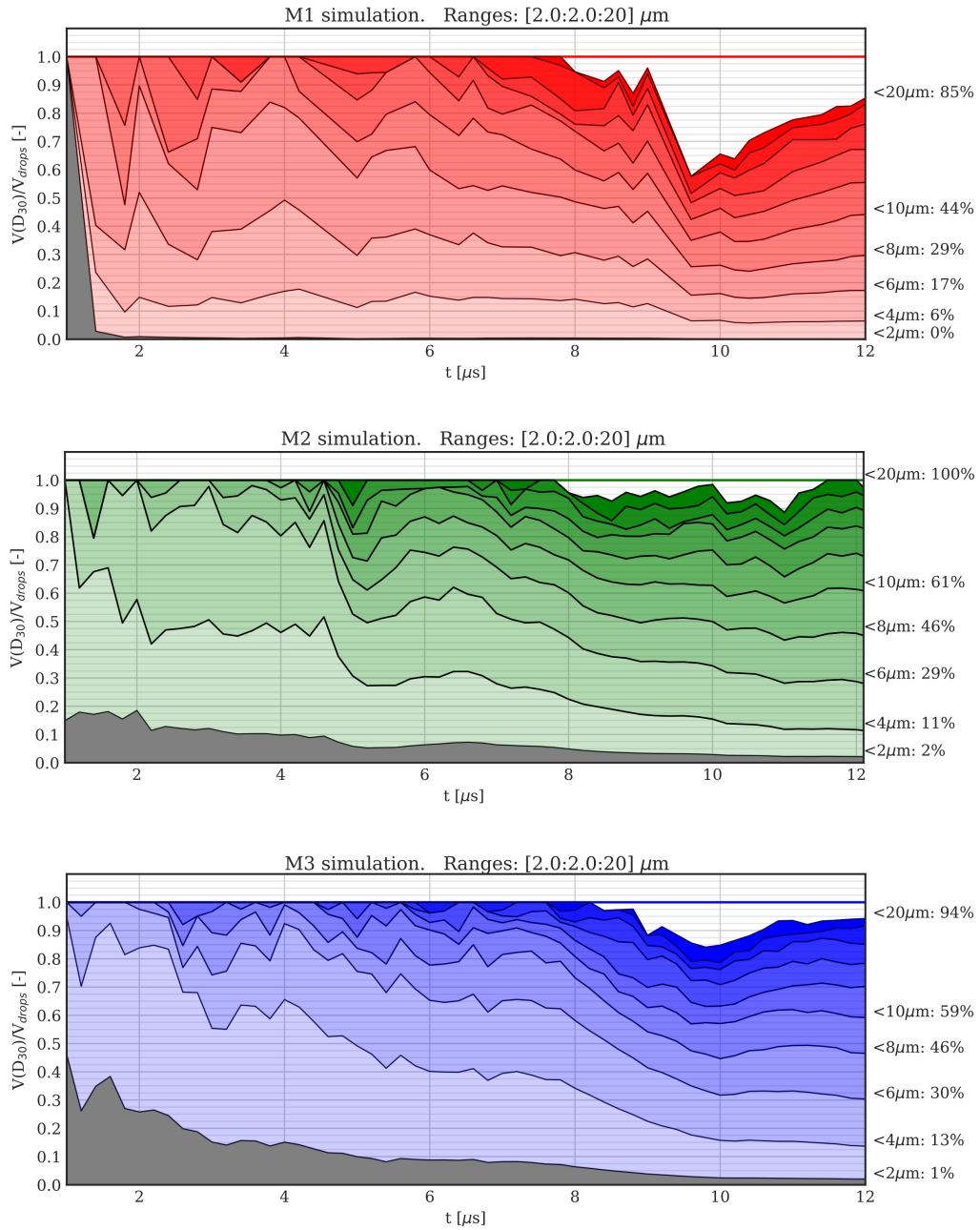


Figure 13: Evolution in time of the cumulative distribution functions of the three simulations M1(red), M2(green), and M3(blue). The drops are grouped in ranges from 0 to 20 μm with a width of 2 μm . The first group of drops ($D_{30} \in (0, 2)\mu\text{m}$) is gray colored to highlight that it contains the under-resolved drops. The right side of each graph shows the cumulative volume fractions at 12 μs .

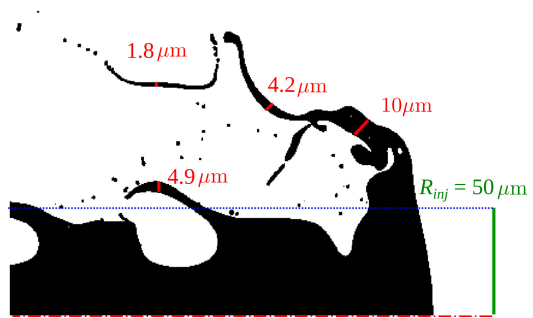


Figure .14: Sheet thickness measurement over VOF field with on the M3 simulation.