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A Σ -Y two-fluid model with dynamic local topology detection: Application to high-speed droplet impact

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Abstract

A numerical methodology resolving flow complexities arising from the coexistence of both multi-scale processes and flow regimes is presented. The methodology employs the compressible Navier-Stokes equations of two interpenetrating fluid media using the two-fluid formulation; this allows for compressibility and slip velocity effects to be considered. On-the-fly criteria switching between a sharp and a diffuse interface within the Eulerian-Eulerian framework along with dynamic interface sharpening is developed, based on an advanced local flow topology detection algorithm. The sharp interface regimes with dimensions larger than the grid size are resolved using the VOF method. For the dispersed flow regime, the methodology incorporates an additional transport equation for the surface-mass fraction (Σ -Y) for estimating the interface surface area between the two phases. To depict the advantages of the proposed multiscale two-fluid approach, a high-speed water droplet impact case has been examined and evaluated against new experimental data; these refer to a millimetre size droplet impacting a solid dry smooth surface at velocity as high as 150m/s, which corresponds to a Weber number of $\sim 7.6 \times 10^5$. Droplet splashing is followed by the formation of highly dispersed secondary cloud of droplets, with sizes ranging from 10^{-5} mm close to the wall to less than $1\mu\text{m}$ forming at the later stages of droplet fragmentation. Additionally, under the investigated impact conditions, compressibility effects dominate the early stages of droplet splashing. A strong shock wave forms and propagates inside the droplet, where transonic Mach numbers occur; local Mach numbers up to 2.5 are observed for the expelled surrounding gas outside the droplet. Relative velocities between the two fluids are also significant; local values on the tip of the injected water film up to 5 times higher than the initial impact velocity are observed. The proposed numerical approach is found to capture relatively accurately the flow phenomena and provide additional information regarding the produced flow structure dimensions, which is not available from the experiment.

Keywords: two-fluid model; compressible Navier-Stokes; Σ -Y formulation; supersonic flow; adaptive flow topology detection; droplet impact

1. Introduction

Multiscale complexities are realised in numerous multiphase flow fields of both industrial and more theoretical interest due to the temporal and spatial geometric diversity of the flow patterns formed by the interacting phases. The different flow structures are characterized by a broad range of scales which as a result, impose the coexistence and dynamic transition between different flow regimes (Kolev, 2007). Examples from the plethora of multidisciplinary applications include fuel spray injection in internal combustion engines, droplet aerodynamic-induced breakup occurring in all type of liquid-fuel combustors (Theofanous, 2011), droplet splashing (Moreira, Moita and Panão, 2010), bubble column bioreactors for chemical processes (Schügerl and Bellgardt, 2000) and even the Rayleigh–Taylor instability in a supernova explosion (Sharp, 1983). With regards to the two-phase flow of a liquid

46 and a gaseous phase, macroscales dominate the free surface regions, where the two phases are
47 separated with a well-defined interface in the presence of a segregated regime (Ishii and Hibiki, 2011),
48 while flow regions with an intense fluid dispersity due to the dominance of fluid microparticles
49 indicate a dispersed regime (Ishii and Hibiki, 2011). Adding to the complexities imposed by the scale
50 heterogeneity of the flow field, the simultaneous presence of different regimes comes with additional
51 limitations arising from the different physical factors influencing them; surface tension effects
52 dominate the segregated flow, while aerodynamic forces play the dominant role in the dispersed flow
53 regions. Thus, under the scope of a mathematical modelling, it remains challenging and
54 computationally demanding to deal with such multiscale flow systems and simultaneously account for
55 different scaled structures, governed by different physical scales that cannot be captured by the grid
56 resolution available.

57 Several numerical approaches have been proposed in the literature over the years, regarding the
58 modelling of multiphase flows in engineering applications. Among the most classic models is the
59 Discrete Droplet Method (DDM) (Dukowicz, 1980), in which the dispersed phase is considered as a
60 number of similar physical droplets within a stochastic Lagrangian framework; the conservation
61 equations are solved for the Eulerian continuous phase. Even though the DDM method has been
62 widely utilised in different applications (see selectively (Berlemont, Desjonqueres and Gouesbet,
63 1990), (Boileau *et al.*, 2008), (Gorokhovski and Saveliev, 2003)), it is generally valid only when the
64 liquid volume fraction is relatively small and the droplets are homogeneously distributed, introducing
65 remarkable limitations in many simulations. In the context of an exclusively Eulerian approach, the
66 homogeneous mixture model (Drew, 1983) is based on the assumption of a single velocity field for
67 both the dispersed and the continuous phases. Due to the simple mathematical formulation and the
68 computational feasibility in liquid fuel spray injection applications under realistic geometries and
69 operating conditions (Koukouvinis *et al.*, 2016), (Pei *et al.*, 2015), the homogeneous mixture model
70 has been implemented and extensively used in both open-source and commercial software. However,
71 the deficiencies regarding the two-phase mixture assumption, the interface diffusivity and the
72 absence of physical sub-grid scale models, often restrict the physical consistency of the obtained
73 results. Under a fully Eulerian formulation, the inhomogeneous mixture model (Ishii and Mishima,
74 1984), often referred to as the multifluid model, is another alternative approach in which each of the
75 interpenetrating phases is considered separately with a different set of conservation equations;
76 numerical modelling of the mass, momentum and energy exchange mechanisms is required for
77 simulating the interactions between them. Nevertheless, the Eulerian-Eulerian approach provides
78 more accurate results mainly under highly dispersed conditions away from regimes where a dispersed
79 phase cannot be distinguished (Rusche, 2002).

80 In an attempt to overcome the limitations of the previous models and improve the accuracy of
81 multiphase flow simulations, Direct Numerical Simulations (DNS), which correspond to a full-scale
82 analysis of the local variable topology without any assumptions or additional numerical models
83 introduced, are the optimum numerical tool. However, very few DNS or unresolved-DNS studies can
84 be found in the literature (selectively (Rossinelli *et al.*, 2013), (Gorokhovski and Herrmann, 2008),
85 (Herrmann, 2010), (Shinjo and Umemura, 2010), (Shinjo and Umemura, 2011)), particularly for
86 industrial applications; this is due to the prohibitive computational cost with the current
87 computational capabilities. Focusing specifically on improving the representation of the liquid gas
88 interface, several interface capturing and interface tracking methods have been proposed with the
89 volume of fluid (VOF) method (Hirt and Nichols, 1981), (Scardovelli and Zaleski, 1999), the level-set
90 method (Osher and Fedkiw, 2006), (Sethian, 1996), the ghost-fluid method (Fedkiw *et al.*, 1999) and
91 the front-tracking method (Unverdi and Tryggvason, 1992), (Tryggvason *et al.*, 2002) to be commonly
92 used. A sharp interface approach can be applicable in segregated flows, where large-scale flow

93 features are dominant and the local interfacial structures can be well resolved under the requirement
94 of a sufficiently fine computational mesh. Thus, an interface sharpening formulation in dispersed flow
95 regions with occurring micro- or even nanoparticles is not computationally feasible.

96 Recently, more advanced numerical models have been developed in order to overcome the
97 dependency on local flow regimes in specific multiphase flow applications. The ELSA model (Vallet,
98 Burluka and Borghi, 2001) is based on the principles of the Σ -Y model (Vallet and Borghi, 1999), which
99 was initially proposed for simulating the flame surface area evolution in combustion simulations
100 (Marble and Broadwell, 1977); it provides a dynamic transition between a Eulerian and a Lagrangian
101 framework in the primary and secondary liquid spray atomization regions, respectively. The additional
102 transport equation for the liquid gas interface surface area density (Σ) allows for representation of
103 unresolvable sub-grid scale structures with a viable computational cost, ought to the physical
104 modelling of the mechanisms responsible for the interface surface area density formation (Lebas *et al.*,
105 2009). Several variations and improvements of the original ELSA model have been proposed so far,
106 including vaporisation (Lebas *et al.*, 2009) and slip-velocity effects (Andreini *et al.*, 2016), as well as a
107 sharp interface formulation in the Eulerian part of an atomizing spray (Anez *et al.*, 2018). A further
108 insight into the sub-grid scale phenomena can be gained with the implementation of a probability
109 density function (PDF) so as to obtain secondary droplet size distributions and other stochastic
110 properties of the dilute spray using the Method of Moments (Marchisio *et al.*, 2003), (Marchisio *et al.*,
111 2003). In one of the most recent formulations, a joint sub-grid scale volume surface PDF (Navarro-
112 Martinez, 2014) is introduced for the liquid surface and volume dependence to predict in more detail
113 the interface surface area density production and destruction at sub-grid level within the ELSA model
114 (Vallet, Burluka and Borghi, 2001). With respect to commercial CFD codes, a complete atomization
115 model for liquid fuel spray simulations has been integrated in AVL FIRE® (AVL, 2013), using a fully
116 Eulerian formulation. The interacting phases are resolved with the incorporation of a specific number
117 of Eulerian droplet classes, which share the same properties (Vujanović *et al.*, 2015). Moreover, in the
118 recent versions of OpenFOAM®, a hybrid fully Eulerian incompressible solver has been implemented,
119 namely multiphaseEulerFoam (Wardle and Weller, 2013) and used in multiscale vertical plunging jets
120 (Shonibare and Wardle, 2015), supporting a dynamic switching between a diffuse and a sharp
121 interface approach within the same multifluid framework. However, the advantages of the state-of-
122 the-art numerical models over the more classic approaches are restricted to the needs of the specific
123 applications for which they were developed. Therefore, there is a gap in the literature for a holistic
124 numerical approach, which can be applicable in any flow field governed by a multiscale character and
125 complex physical phenomena, including high compressibility and slip velocity effects, regardless of the
126 limitations of local flow characteristics.

127 The above methodologies can be applied to the case of a droplet impacting on solid surfaces, which
128 represents a fundamental multiscale flow problem, that still attracts the scientific interest, due to its
129 relevance in many engineering applications, such as cooling, coating, inkjet printing, fuel injection in
130 internal combustion engines, as it is stated in the review works of (Kandlikar and Bapat, 2007),
131 (Moreira, Moita and Panão, 2010). The droplet deformation and potential fragmentation after impact
132 is very sensitive to several parameters regarding the impact and target conditions; namely the impact
133 velocity, the droplet initial diameter and physical properties, target wettability, roughness and surface
134 temperature, as it has been investigated in numerous experimental studies (see selectively (Pan,
135 Tseng and Wang, 2010), (Visser *et al.*, 2012), (Antonini, Amirfazli and Marengo, 2012), (Roisman,
136 Lembach and Tropea, 2015), (Liang and Mudawar, 2017)). The post-impact outcomes are subject to
137 different regimes, ranging from spreading or even sticking on the surface to rebounding and splashing
138 and they have been comprehensively presented in the literature (Rein, 1993), (Yarin, 2006), (Josserand
139 and Thoroddsen, 2016) and illustrated on regime maps as a function of dimensionless impact

140 parameters (Ma *et al.*, 2017), (Bertola, 2015). Several correlations to define the splashing regime
141 threshold have been established (Yarin and Weiss, 1995), (Range and Feuillebois, 1998), while the
142 most widely used criterion for the transition between the deposition and splashing regimes under
143 large impact velocities is the parameter of Mundo (Mundo, Sommerfeld and Tropea, 1995), which is
144 based on the Weber and Ohnesorge numbers. Additionally, conducted experimental studies have
145 been utilised for the development of empirical models, corresponding to the droplet post-impact
146 characteristics under the influence of different impact regimes, as it is thoroughly described in (Cossali,
147 Santini and Marengo, 2005), in order to provide numerical models for spray impingement simulations.

148 Even though the single droplet impact onto solid surfaces has been extensively investigated with
149 experimental studies since 1877 (Worthington, 1877), the mechanisms of the prompt and violent
150 splashing under high impact velocities, which correspond to the massive spatial dispersion of the
151 produced secondary droplets far away from the solid surface and the dominance of compressibility
152 phenomena with strong propagating shock waves inside the deforming droplet, have not been
153 precisely revealed yet. Due to the limitation of the high speeds and small structures involved, recent
154 advancements in imaging technologies (Thoroddsen, Etoh and Takehara, 2008) have contributed to
155 the performance of new experiments under higher impact velocities. In (Xu, Zhang and Nagel, 2005)
156 the corona splashing of an ethanol droplet on a dry and smooth surface with impact Weber number
157 equal to 1685 was examined; the created lamella reached a maximum spreading velocity of 30m/s. In
158 (Visser *et al.*, 2015) experiments with water microdroplets have been conducted, impacting on both
159 hydrophilic and hydrophobic surfaces with velocities up to 50m/s and Weber numbers that do not
160 exceed the value of 1770. However, despite the high speed conditions, no splash but only spreading
161 of the droplet on the surface was observed, due to the influence of the surrounding air. One of the
162 few and most recent experiments in which a prompt splashing was illustrated is the work of
163 (Thoroddsen, Takehara and Etoh, 2012), in which a water droplet was subject to an impact with a
164 smooth and solid surface at Weber numbers up to 2480, followed by the creation of water
165 microdroplets with maximum spreading velocity of 100m/s. Finally, in (Field, Dear and Ogren, 1989)
166 an experiment of high speed droplet impact at 110m/s was performed, with emphasis put on
167 capturing the propagating shock wave inside the droplet at the early stages of the impact with the
168 target, without examining the later splashing effects. Thus, it is noticeable from the literature that
169 high-speed droplet impact experiments are limited; available studies do not exceed Weber number
170 values of 2500 and they mainly focus on the early stages of the droplet and wall interaction.

171 Regarding the numerical investigation of droplet impact cases, most recent studies examine the
172 impact on solid surfaces under the spreading (Margarinos *et al.*, 2014), (Visser *et al.*, 2015) or the
173 corona splashing (Guo, Lian and Sussman, 2016), (Wu and Cao, 2017) regimes; they utilise an interface
174 capturing method for the conducted simulations. With the VOF method to be the most commonly
175 used approach, the droplet deformation and spreading on the target can be captured in detail with a
176 sufficiently fine mesh. However, in the case of higher impact velocities, which result to splashing and
177 fragmentation of the droplet into secondary microscale structures, the performed simulations are
178 restricted to the early stages of the phenomena since the later stages of droplet fragmentation are
179 dominated by computationally prohibitive scales for a VOF simulation. Thus, a more advanced
180 numerical modelling is required to deal simultaneously with the early and later stages of the splashing
181 droplet evolution. Moreover, other studies perform high-speed droplet impact simulations with the
182 focus on capturing the occurring compressibility phenomena (Haller *et al.*, 2002), (Niu and Wang,
183 2016), (Kyriazis, Koukouvinis and Gavaises, 2018), (Wu, Xiang and Wang, 2018) namely the strong
184 shock waves inside the droplet and the produced cavitation regions, which are formed and dominate
185 during the early stages of the impact, excluding in this manner the secondary droplet dispersion from
186 the scope of their numerical investigation.

187 Following the limitations of the currently used numerical methodologies in multiscale flow
188 applications, the present study proposes a new numerical framework which has been developed in
189 OpenFOAM® utilising the two-fluid formulation (Ishii and Mishima, 1984); this allows for both
190 compressibility and slip velocity effects to be taken into account. The model solves for an additional
191 transport equation for the interface surface area density; the previously developed Σ -Y model (Vallet
192 and Borghi, 1999) for incompressible flows is coupled here for the first time with a compressible two-
193 fluid framework. This provides significant information for the unresolved sub-grid scale phenomena,
194 which are related to the interface formation during the flow development. The Σ -Y two-fluid model is
195 also combined with a dynamic switching between the sharp and the diffuse interface approaches that
196 co-exist during the numerical solution at different parts of the computational domain. Thus, it is
197 possible to deal simultaneously with the segregated and the dispersed flow regions; the two-fluid
198 model formulation has been coupled with the VOF method to operate under the segregated flow
199 regime. The dynamic switching is performed with an advanced topology detection algorithm relative
200 to criteria available in the literature (Wardle and Weller, 2013), (Anez *et al.*, 2018). However, apart
201 from the numerical limitations of the VOF and the diffuse interface approaches with respect to the
202 computational mesh which correspond to the commonly used switching criteria, the proposed flow
203 topology detection algorithm also evaluates the local flow characteristics. The developed
204 methodology is initially validated against a shock tube problem and a rising bubble. Following,
205 validation is performed against the challenging case of a high-speed droplet impact, using new
206 experimental data obtained specifically for this case. These refer to impact Weber number of the order
207 of 10^5 , which is much higher than the available up-to-date literature. Finally, emphasis from the
208 numerical perspective is given on providing an insight into the dispersed regions of the flow field at
209 the later stages of the droplet fragmentation evolution, where even the experimental investigation
210 cannot contribute with sufficient information due to limitations in diagnostic methods for high Mach
211 number flows consisting of a large number of droplets with sizes less than $1\mu\text{m}$.

212 2. Numerical Model

213 The Σ -Y two-fluid model with dynamic local topology detection has been implemented in OpenFOAM®
214 with further developments on twoPhaseEulerFoam solver, an available compressible Eulerian
215 pressure-based solver. In principle, the numerical model consists of the same set of governing
216 equations for both multiscale formulations, namely the sharp and the diffuse interface approach, with
217 specific source terms to be activated and deactivated depending on the currently operating
218 formulation of the solver, as it is described in detail below.

219 2.1. Two-Fluid Model Governing Equations

220 In the context of a two-fluid approach (Ishii and Mishima, 1984), the volume averaged conservation
221 equations governing the balance of mass, momentum and energy are solved separately for each phase
222 k :

$$223 \quad \frac{\partial}{\partial t} (a_k \rho_k) + \nabla \cdot (a_k \rho_k u_k) = 0 \quad (1)$$

$$224 \quad \frac{\partial}{\partial t} (a_k \rho_k u_k) + \nabla \cdot (a_k \rho_k u_k u_k) = -a_k \nabla p + \nabla \cdot (a_k \tau_k^{eff}) + a_k \rho_k g + \sum_{\substack{n=1 \\ n \neq k}}^2 M_{kn} \quad (2)$$

$$225 \quad \frac{\partial}{\partial t} [a_k \rho_k (e_k + k_k)] + \nabla \cdot [a_k \rho_k (e_k + k_k) u_k] = -\nabla \cdot (a_k \mathbf{q}_k^{eff}) - \left[\frac{\partial a_k}{\partial t} p + \nabla \cdot (a_k u_k p) \right] \\ 226 \quad + a_k \rho_k g \cdot u_k + \sum_{\substack{n=1 \\ n \neq k}}^2 E_{kn} \quad (3)$$

227 The numerical method is based on a finite-volume framework, using an implicit pressure-based solver
228 for the governing equations of the two-fluid model. Numerical coupling for the independent systems
229 of conservation equations is achieved through additional source terms added to the Navier-Stokes
230 equations, which appear after the imposed averaging procedure. These source terms account for the
231 mass, momentum and energy exchange phenomena by providing suitable closure relations for the
232 macroscopic interfacial interactions occurring in a transient multiphase flow system. Specifically, the
233 interfacial momentum source term M_{kn} represents the forces acting on the dispersed phase and
234 depends on local topology, since different forces are dominant under different flow regimes. The
235 interfacial energy source term E_{kn} demonstrates the heat transfer between the phases that can be
236 modelled via a standard heat transfer law. The interfacial mass source term, which is responsible for
237 the mass transfer due to phase-change effects or other interfacial phenomena that result to
238 production or destruction of the interface, such as sub-grid scale turbulence and droplet interactions,
239 is not implemented in the continuity equations as expected. Instead, in the present work the mass
240 exchange contributions with an effect on interface formation are considered in the transport equation
241 for the liquid gas interface surface area density. Phase-change phenomena, like vaporisation and
242 cavitation, are neglected since they are negligible in the examined high-speed droplet impact case at
243 the early stages of impact, where temperature variation around the standard conditions is not
244 significant and local pressure drop is not sufficient to cause remarkable cavitation regions, as it has
245 been stated before in the literature for similar impact conditions (Niu and Wang, 2016), (Kyriazis,
246 Koukouvinis and Gavaises, 2018).

247 Viscous and turbulence effects are introduced in the model with the effective stress tensor τ^{eff} in the
248 momentum equations and the effective heat flux vector q^{eff} in the energy equations; τ^{eff} accounts for
249 the molecular viscosity and the Reynolds stress tensor, which based on Boussinesq's hypothesis
250 relates turbulent velocity fluctuations to the eddy viscosity (Boussinesq, 1877); q^{eff} corresponds to the
251 laminar and turbulent thermal diffusivity. For the turbulent components, appropriate models are
252 implemented within either a RANS or an LES framework in OpenFOAM®; LES modelling is used for the
253 turbulent flow cases in the present study with the implementation of the one-equation SGS model
254 (Lahey, 2005). Given the occurring Reynolds numbers, a dimensionless wall distance y^+ with a value
255 lower 1 is observed; thus, the appropriate turbulent wall functions are implemented for capturing the
256 near-wall phenomena; the two-layer wall function is used which is a blending between the logarithmic
257 and the linear laws for the turbulent and viscous sublayers, respectively.

258 Finally, the thermodynamic closure of the system is achieved by solving independently an individual
259 equation of state for each phase from which the corresponding density field is obtained. In the
260 following simulations, the ideal gas equation of state is used for the gaseous phase and the stiffened
261 gas equation of state (Ivings, Causon and Toro, 1998) has been implemented and used for the liquid
262 phase. The stiffened gas equation of state is basically the same as the ideal gas equation of state with
263 an additional pre-pressurization term to match the density and stiffness of the liquid. Despite its
264 deficiencies, it is commonly used in fundamental studies (Saurel, Petitpas and Abgrall, 2008) and highly
265 violent phenomena (Beig, Aboulhasanzadeh and Johnsen, 2018); moreover, it is known to be valid for
266 the pressure and temperature conditions examined here.

267 Σ -Y Model Transport Equations:

268 The liquid dispersion in a liquid and gaseous flow is simulated with the liquid phase volume fraction
269 transport equation, which represents the volume proportion of liquid at a given volume in the
270 computational domain. The transport equation for the liquid volume fraction in a compressible two-
271 phase flow is:

$$272 \quad \frac{\partial a_l}{\partial t} + \nabla \cdot (a_l u_m) + v_{topo} [\nabla \cdot (a_l (1 - a_l) u_c)] = a_l a_g \left(\frac{\psi_g}{\rho_g} - \frac{\psi_l}{\rho_l} \right) \frac{Dp}{Dt} + a_l \nabla \cdot u_m - (1 - v_{topo}) R_{a_l} \quad (4)$$

273 where the topological parameter v_{topo} allows for distinguishing between the two different interface
 274 approaches by taking either 0 or 1 value under a diffuse or sharp interface formulation respectively.
 275 u_c is the artificial compression velocity (Deshpande, Anumolu and Trujillo, 2012) that is introduced
 276 along the interface as a countereffect of the inevitable numerical diffusion in order to maintain
 277 interface sharpness in flow regions subject to a segregated regime. The turbulent liquid flux R_{a_l} (Vallet,
 278 Burluka and Borghi, 2001) on the RHS of the transport equation accounts for the liquid dispersion
 279 induced by turbulent velocity fluctuations, which is important in dispersed flows and smaller scales.
 280 Additionally, since a compressible flow is involved, the gradients of liquid density that are related to
 281 compressibility effects on the liquid volume fraction are taken into consideration (Jadidi *et al.*, 2014).

282 The liquid gas interface surface area density, namely the surface area of the liquid gas interface per
 283 unit of volume, provides supplementary information regarding the interface formation without the
 284 assumption of a particular shape in the produced flow features. The transport equation for the liquid
 285 gas interface surface area density (Lebas *et al.*, 2009) is described as follows:

$$286 \quad \frac{\partial \Sigma'}{\partial t} + \nabla \cdot (\Sigma' u_m) = (1 - v_{topo}) \left[-R_\Sigma + C_{SGS} \frac{\Sigma}{\tau_{SGS}} \left(1 - \frac{\Sigma}{\Sigma_{SGS}^*} \right) \right] \quad (5)$$

287 The turbulent flux of the interface surface area density R_Σ , namely the first source term on the RHS of
 288 the transport equation, represents the surface area diffusion due to turbulent velocity fluctuations.
 289 The second source term on the RHS accounts for all physical mechanisms which fall below the
 290 computational mesh resolution and are responsible for the surface area production and destruction.
 291 In sharp interface regions with dominant large scale features the evolution of the interface surface
 292 area is captured directly by the computational model and grid. On the contrary, in highly diluted and
 293 dispersed flows, the interface production and destruction at sub-grid level affects significantly the
 294 overall interface formation; thus, appropriate modelling is required to obtain this sub-grid scale
 295 information. Under the assumption of a minimum interface surface area due to simultaneous
 296 existence of liquid and gas on the interface (Chesnel *et al.*, 2011), the total interface surface area
 297 density is defined as:

$$298 \quad \Sigma = \Sigma' + \Sigma_{min} \quad (6)$$

299 where Σ_{min} is the minimum interface surface area density that can be found within a control volume
 300 for a given liquid volume fraction value with $0 < \alpha_l < 1$, which imposes the presence of two phases and
 301 thus, the presence of an interface in the examined control volume. Based on empirical correlations
 302 obtained from CDNS studies and under the assumption of a spherical droplet inside the examined
 303 computational cell, Σ_{min} is defined as $\Sigma_{min} = 2.4 \sqrt{a_l (1 - a_l)} V_{sphere}^{-1/3}$ (Chesnel *et al.*, 2011).

304 2.2. Sharp Interface Approach

305 Interface sharpening is implemented in OpenFOAM® with the MULES algorithm (Deshpande, Anumolu
 306 and Trujillo, 2012), an iterative technique which guarantees boundness of the volume fraction and
 307 sharpness at the interface by modifying the advection term in the transport equation for the volume
 308 fraction. In this manner, an additional advection term is introduced which acts as an artificial
 309 compression in order to maintain sharpness without the need for interface reconstruction. This
 310 approach has been implemented within the proposed multiscale two-fluid framework and thus in the
 311 segregated flow regions the transport equation for the liquid volume fraction takes the final form of

312 equation (4) with the topological parameter v_{topo} set to 1. Then, the artificial compression velocity u_c
 313 is given by the expression:

$$314 \quad u_c = C_\alpha |u_m| \frac{\nabla a_l}{|\nabla a_l|} \quad (7)$$

315 with C_α the interface compression parameter that takes values equal or greater than 1 so as to increase
 316 the imposed interface sharpness. In the following simulations the typical value of $C_\alpha=1$ has been
 317 implemented so as to introduce interface sharpness with the MULES algorithm.

318 However, the introduction of an interface sharpening approach within a two-fluid framework requires
 319 further modifications in the numerical model. In the limit of a sharp interface, the velocities on either
 320 side of the interface must be equal in order to eliminate the relative velocity and meet the no-slip
 321 interface condition. At the same time, a fundamental principle of the two-fluid model is the presence
 322 of separate velocity fields for the two interpenetrating liquids. Several studies in the literature (Černe,
 323 Petelin and Tiselj, 2001), (Wardle and Weller, 2013), (Strubelj and Tiselj, 2011) are dealing with the
 324 coupling of a two-fluid model and an interface sharpening method by implementing an additional
 325 source term in the momentum equations. This extra term practically imposes large interfacial drag
 326 values; as a result, the relative velocity on the interface is eliminated and finally the coupling between
 327 the two-fluid model and the sharp interface approach is stabilized. In the present model the source
 328 term introduced in the momentum equations (2) has an expression similar to the aerodynamic drag
 329 force (Strubelj and Tiselj, 2011) and enforces instantaneous equalizing of the velocities near the
 330 resolved interface. The artificial drag force is defined as:

$$331 \quad F_{Da} = v_{topo} F(u_r) \frac{\tau_r}{\Delta t} \quad (8)$$

332 where $F(u_r)$ is an expression proportional to the relative velocity u_r between the two phases and the
 333 density of the two-fluid mixture ρ_m with $F(u_r) = a_l(1 - a_l)u_r\rho_m$ as proposed by (Strubelj and Tiselj,
 334 2011), Δt the computational time step and τ_r a relaxation factor which needs to be calibrated
 335 correspondingly, in order to meet the no-slip interface condition. As it is described in detail in
 336 paragraph 3.2, the elimination of the interfacial relative velocity, which practically results to a stronger
 337 coupling between the two-fluid model and the sharp interface approach, is achieved by maximizing
 338 the relaxation factor τ_r . In an attempt to avoid any case-dependent calibration of τ_r , an on-the-fly
 339 algorithm has been developed which gradually increases the value of τ_r starting from the value of 1,
 340 until the point that the tangential component of the relative velocity on the interface reaches a
 341 sufficiently low lower-bound close to zero; under this condition, the no-slip interface condition is
 342 satisfied. In practice, a numerical criterion is examined on the interface, which requires for the
 343 tangential component of the relative velocity to be only a small proportion of the total local relative
 344 velocity, approaching a zero value.

345 Under a segregated flow regime, the surface tension plays a greater role against the aerodynamic
 346 forces. Therefore, its contribution should be taken into consideration and a surface tension force is
 347 added as a source term in the momentum equations (2). The surface tension force is defined by the
 348 Continuum Surface Force (CSF) (Brackbill, Kothe and Zemach, 1992) as:

$$349 \quad F_s = v_{topo} \sigma \kappa \frac{\nabla \rho}{[\rho]} \frac{\rho}{\langle \rho \rangle} \quad (9)$$

350 where σ is the surface tension coefficient, κ the interface curvature, $[\rho]$ the density jump described as
 351 $[\rho]=\rho_g-\rho_l$ and $\langle \rho \rangle$ the density at the interface given by $\langle \rho \rangle = \frac{1}{2}(\rho_l + \rho_g)$ in order to replace the local
 352 discontinuity with a smooth variation.

353 Regarding the interface density, all sub-grid scale phenomena, which are modelled via source terms
 354 in equation (5), are out of the scope of a sharp interface approach and thus, the RHS of the transport
 355 equation is set to zero. Besides, a basic principle of the multiscale formulation is the accurate
 356 topological distinction between different flow regimes and the imposition of a sharp interface
 357 approach in regions where all present flow features can be resolved by the grid resolution used.

358 2.3. Diffuse Interface Approach

359 Under a dispersed flow regime with prevailing small dispersed structures, the aerodynamic forces and
 360 particularly the drag force acting on the dispersed phase is the dominant factor in interfacial
 361 momentum exchange between the liquid and gaseous phases. Different drag models are implemented
 362 depending on local flow conditions (Marschall, 2011), i.e. dispersed droplets in continuous gas or
 363 dispersed bubbles in continuous liquid. The drag force, which is introduced as the interfacial
 364 momentum source term in momentum equations (2), is described as:

$$365 F_D = (1 - v_{topo}) \frac{1}{2} C_D \rho_{continuous} u_r |u_r| A_{particle} \quad (10)$$

366 where $\rho_{continuous}$ is the density of the phase, which is considered continuous and $A_{particle}$ is the projected
 367 area of a typical dispersed particle. For the estimation of the drag coefficient C_D , there are many
 368 empirical models in the literature (Schiller and Naumann, 1933), (Ishii and Zuber, 1979), (Tomiyama
 369 and Shimada, 2001) depending on properties of the flow field and the discrete particle characteristics.
 370 In the present work, where the focus is mainly on the motion of very small droplets in highly dispersed
 371 flows with low or moderate Reynolds numbers, C_D is obtained from the model of Rodi and Fueyo
 372 (Kelbaliyev, 2011):

$$373 C_D = \begin{cases} \frac{16}{Re}, & Re < 1.5 \\ \frac{14.9}{Re^{0.78}}, & 1.5 < Re \leq 80 \\ \frac{49.9}{Re} \left(1 - \frac{2.21}{Re^{0.5}}\right) + 1.17 \times 10^{-8} Re^{2.615}, & 80 < Re \leq 1530 \\ 2.61, & Re > 1530 \end{cases} \quad (11)$$

374 However, since many semi-empirical correlations are involved, the closure relations of the interfacial
 375 source terms are usually the main cause for the uncertainties of the two-fluid model. In an attempt to
 376 reduce the possible inaccuracies, in the proposed numerical model the interface surface area is
 377 obtained from the transport equation for the interface surface area density, which is used to calculate
 378 a characteristic length corresponding to the flow structures in each computational cell. More
 379 specifically, the diameter of a spherical particle which has the same volume to surface area ratio as
 380 the examined computational cell volume to the calculated interface surface area density, is used as
 381 the equivalent dispersed particle diameter in drag force calculations. Then, the interface surface area
 382 density diameter can be defined as follows (Chesnel *et al.*, 2011):

$$383 d_\Sigma = \frac{6a_l(1-a_l)}{\Sigma} \quad (12)$$

384 Concerning the transport equation for the liquid volume fraction, the diffuse interface approach
 385 results to exclusion of the interface compression term; consideration of the sub-grid turbulent
 386 fluctuations, as it appears in equation (4) with the topological parameter v_{topo} , is set to 0. The turbulent
 387 liquid flux R_{al} (Vallet, Burluka and Borghi, 2001) on the RHS of the transport equation represents
 388 stochastic liquid dispersion phenomena due to the occurring turbulence. Previous studies on
 389 modelling R_{al} (Demoulin *et al.*, 2007), (Andreini *et al.*, 2016) depict a relation between the statistically
 390 dependent turbulent velocity fluctuations and the averaged local relative velocity, which corresponds
 391 to a correlation between slip and drift velocities of the mean flow field, as presented below:

$$392 \quad R_{a_l} = -\nabla \cdot (\widetilde{a_l'' \rho_l'' u_m''}) = -\nabla \cdot [a_l(1 - a_l)\rho_l V_r] = -\nabla \cdot [a_l(1 - a_l)\rho_l(u_r - V_D)] \quad (13)$$

393 where V_r is the local relative velocity, u_r the slip velocity and V_D the drift velocity. The slip velocity
 394 contribution to the turbulent liquid flux can be calculated directly without the need of modelling due
 395 to the two-fluid formulation. As for the drift velocity effects, they are modelled via a first order closure
 396 (García-Oliver *et al.*, 2013), namely a classic gradient law using the turbulent properties of the liquid
 397 and gaseous mixture.

398 A significant advantage of the proposed multiscale two-fluid formulation is the coupling with the
 399 transport equation for the interface surface area density. Especially within the framework of a diffuse
 400 interface approach, where the interface is neither tracked nor resolved by the grid resolution, this
 401 additional information provides an insight into the interface surface area density evolution in space
 402 and time even in the sub-grid scales. Examining the source terms on the RHS of equation (5), which
 403 are activated under the dispersed regime, the turbulent flux of the interface surface area density R_{Σ}
 404 accounts for its dispersion due to turbulence. Analogous to the turbulent liquid flux R_{a_l} on the RHS of
 405 equation (4), R_{Σ} is a turbulent diffusion term. Then, with respect to the closure of the turbulent liquid
 406 flux R_{a_l} in equation (13), the turbulent diffusion flux R_{Σ} is modelled accordingly (Andreini *et al.*, 2016):

$$407 \quad R_{\Sigma} = -\nabla \cdot (\widetilde{\Sigma' u_m''}) = -\nabla \cdot [\Sigma a_l(1 - a_l)(u_r - V_D)] \quad (14)$$

408 The last term on the RHS of equation (5) represents the sub-grid scale mass exchange phenomena
 409 between the liquid and gaseous phases, which have been neglected from the continuity equations (1)
 410 and are related to the interface surface area density production and destruction. Different physical
 411 mechanisms with an effect on interface formation are included and described by their characteristic
 412 time scale τ_{SGS} , the critical interface surface area density Σ_{SGS}^* at an equilibrium state between
 413 production and destruction of the interface and an adjustable constant coefficient C_{SGS} set to 1 in the
 414 presented cases. In the proposed model, the contributions of turbulent flow stretching and wrinkling
 415 particularly in dense flow regions, the droplet collision and coalescence effects, as well as the
 416 secondary breakup effects of produced droplets are taken into account with the appropriate closure
 417 relations (Lebas *et al.*, 2009) and the implementation of their characteristic time scales τ_{SGS} , which
 418 correspond to the Kolmogorov time scale, the collision time scale obtained from the particle collision
 419 theory and the breakup time scale based on the droplet Weber number, respectively, to be
 420 summarized in Table 1.

421 Table 1 Closure relations for the SGS terms in equation (5) related to interface surface area production and destruction.

SGS mechanism	τ_{SGS}	Σ_{SGS}^*
turbulence	$\frac{k}{\varepsilon}$	$\frac{\alpha_l(1-\alpha_l)\rho_m k_m}{\sigma We_{turb}^*}$ with $We_{turb}^* = 1$ at equilibrium
collision/coalescence	$\frac{1}{\Sigma \sqrt{\frac{2}{3}} k_m}$	$\frac{6\alpha_l(1-\alpha_l)}{d_{\Sigma}^*}$ with $d_{\Sigma}^* = d_{\Sigma} \frac{1 + \frac{We_{coll}^N}{6}}{1 + \frac{We_{coll}}{6}}$ <ul style="list-style-type: none"> • critical We for coalescence: $We_{coll}^N = 12$ • relevant We for collision: $We_{coll} = \frac{4\alpha_l(1-\alpha_l)\rho_l k_m}{\sigma \Sigma}$
secondary breakup	$f(We_{BU}) \frac{d_{\Sigma}}{u_r} \sqrt{\frac{\rho_l}{\rho_g}}$ with $We_{BU} = \frac{6\rho_g u_r^2 \alpha_l(1-\alpha_l)}{\sigma \Sigma}$	$\frac{6\rho_g u_r^2 \alpha_l(1-\alpha_l)}{\sigma We_{BU}^*}$ with $We_{BU}^* = 12(1 + 1.0770h^{1.6}) \cong 12$ for $Oh \ll 1$

422

423 2.4. Flow Topology Detection Algorithm

424 A key factor for the accurate functioning of the multiscale formulation is the implementation of a
425 stable topology detection methodology. The developed algorithm can detect instantaneous
426 topological changes in flow regimes, evaluate the most appropriate numerical treatment for local
427 interfaces and allow for a flexible two-way switching between sharp and diffuse interface approaches.
428 The switching criteria, described in detail below, are applied exclusively in interfacial flow regions as
429 in single phase regions a sharp interface is defined by default.

430 2.4.1. Switching criterion from sharp to diffuse interface approach

431 In any computational cell under the sharp interface approach, a diameter of an equivalent spherical
432 structure based on the curvature of the interface can be calculated as (Shonibare and Wardle, 2015):

$$433 \quad d_{curv} = \frac{2}{\kappa} \quad (15)$$

434 Assuming that at least 3 computational cells are needed for the grid resolution to capture any spherical
435 structure with sufficient sharpness (Shonibare and Wardle, 2015), the following geometric criterion
436 can be proposed as the limit for the sharp interface approach:

$$437 \quad d_{curv} < 3 * \max(d_{cell}) \quad (16)$$

438 Nevertheless, this geometric criterion can only be considered as an indication for a potential switch
439 to a diffuse interface approach. All computational cells which meet criterion (16) are subject to a
440 second stage of topological examination based on the condition of their neighbour cells. The three
441 different possibilities are as follows:

- 442 • A single cell which is supposed to follow a diffuse interface approach based on the geometric
443 criterion but belongs to a strictly segregated region with sharp interfaces, will remain unaffected
444 by changes, as shown in Figure 1(a).
- 445 • When a cell is part of a topologically unstable region, where all its neighbour cells previously
446 respected a sharp interface approach but now some of them are also subject to changes, then as
447 depicted in Figure 1(b), an expanded region is examined. Specifically, the surrounding area of the
448 neighbour cells which are of particular interest is evaluated with regards to the occurring
449 topological conditions. Finally, if the examined cell belongs to a highly transitional region, then the
450 topological criterion is met and a change for the interface approach is applied.
- 451 • As illustrated in Figure 1(c), any cell that is in the border of transition between segregated and
452 highly dispersed flow regimes will follow the tendency of local interface formation and will be
453 subject to the diffuse interface approach in the following time step.

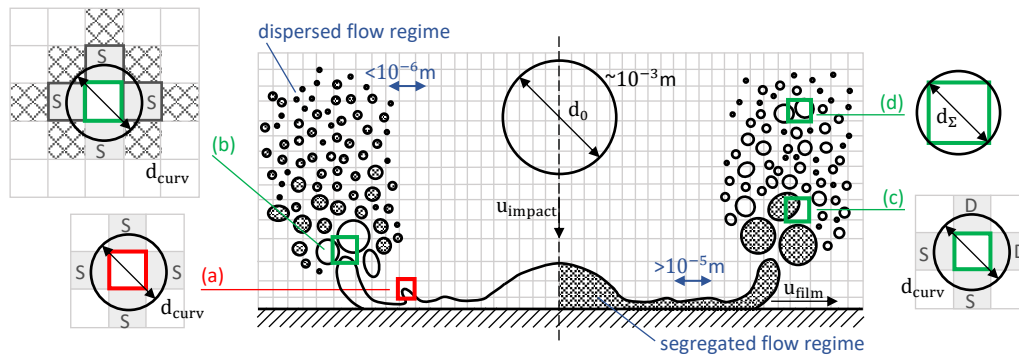
454

455 2.4.2. Switching criterion from diffuse to sharp interface approach

456 The reset of a sharp interface approach for a previously diffuse cell is performed after meeting a single
457 geometric criterion, which correlates the interface surface area density diameter from equation (12)
458 to the local computational mesh resolution. When the calculated diameter d_{Σ} is larger than the cell
459 size, then the presumed dispersed flow features can no longer be treated as mesh unresolvable
460 structures and a switch to a sharpened interface state is required.

$$461 \quad d_{\Sigma} > \min(d_{cell}) \quad (17)$$

462 Since the overall concept of the diffuse interface approach is inextricably linked to sub-grid scale
 463 structures, the described geometric criterion is sufficient for changing the interface formulation
 464 without examining the surrounding flow conditions, as shown in Figure 1(d).



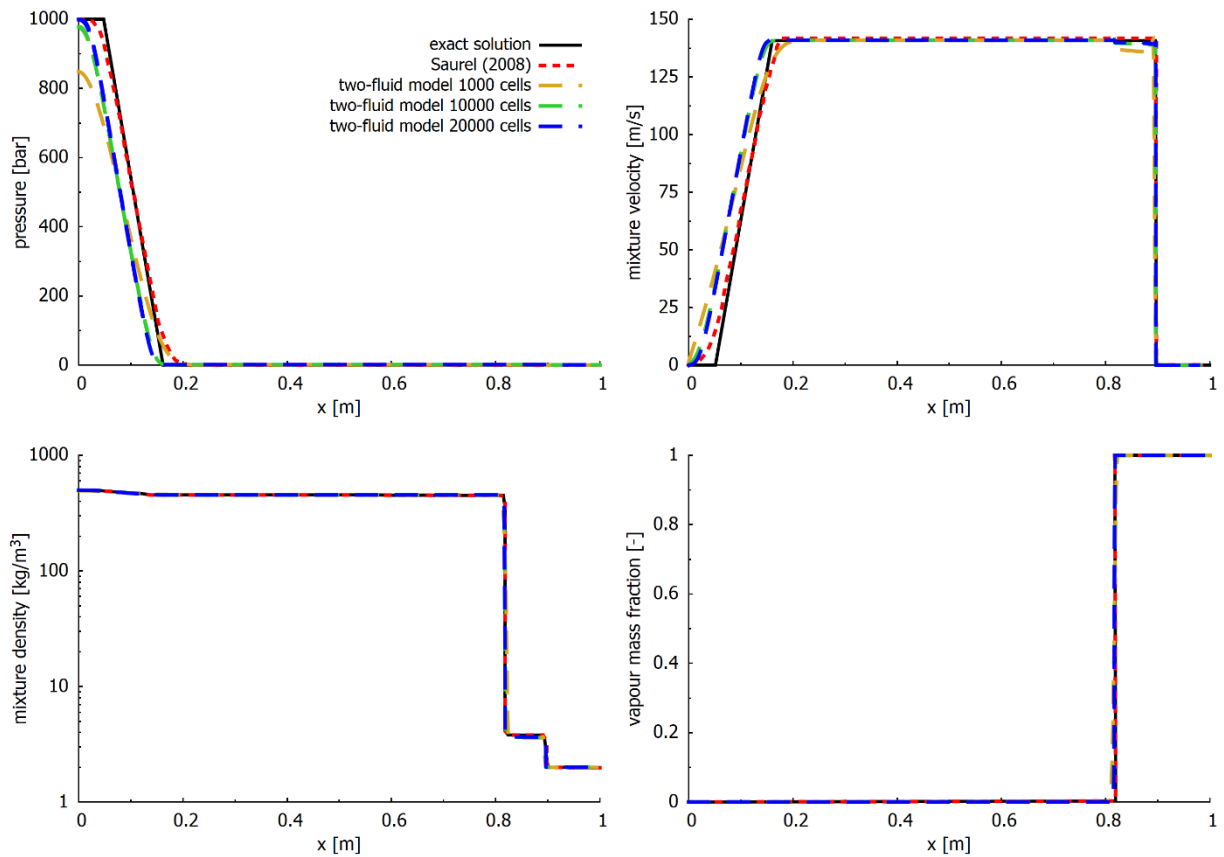
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466 Figure 1 Local topology detection and distinction criteria between the segregated and the dispersed flow regimes in order
 467 to impose the appropriate interface approach in each time step. Application in the multiscale flow of a droplet impact on a
 468 rigid wall with indicative dominant scales under each flow regime.

469 3. Results and Discussion

470 3.1. Two-Phase Shock Tube Problem

471 Initially, the capability of the proposed compressible two-fluid model to capture accurately the wave
 472 dynamics under high density ratios between the interacting phases is examined against the
 473 benchmark case of a two-phase shock tube. A one-dimensional 1m long two-fluid shock tube without
 474 mass transfer and initial discontinuity at $x=0.75\text{m}$, as studied by (Saurel, Petitpas and Abgrall, 2008),
 475 is used for validation. The left part of the shock tube is occupied by liquid dodecane at high pressure
 476 $p_l=10^8\text{Pa}$ and density $\rho_l=500\text{kg/m}^3$, while the right part is set at atmospheric conditions with the
 477 occurring vapour dodecane at density $\rho_v=2\text{kg/m}^3$. The simulation is performed using the
 478 twoPhaseEulerFoam solver in a uniform computational grid of 1000, 10000 and 20000 cells with
 479 second order spatial accuracy and an adaptive time step to meet the convective Courant–Friedrichs–
 480 Lewy (CFL) number of 0.2. As a matter of consistency between the conducted simulation and the
 481 results of (Saurel, Petitpas and Abgrall, 2008) using the hyperbolic two-fluid model with two
 482 temperature and entropy fields but a single pressure and velocity field, the stiffened gas equation of
 483 state with the exact parameters utilised in (Saurel, Petitpas and Abgrall, 2008) has been implemented
 484 in OpenFOAM® and applied for the thermodynamic closure. In Figure 2 the results obtained from the
 485 proposed two-fluid approach and the model of (Saurel, Petitpas and Abgrall, 2008) are compared with
 486 the exact solution at $473\mu\text{s}$ after the initial contact discontinuity was removed. The involved
 487 convectional waves, namely the left-facing rarefaction wave propagating through the liquid dodecane,
 488 the moving from left to right contact discontinuity and the right-facing shock wave propagating through
 489 the vapour dodecane are accurately captured with the proposed two-fluid model. Moreover, the
 490 increase in mesh resolution eliminates the numerical diffusion in the pressure and mixture velocity
 491 fields and the illustrated results using the finest mesh converge to a satisfactory agreement with the
 492 exact solution of the shock tube problem.



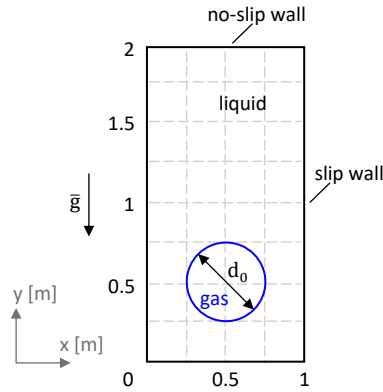
493

494 Figure 2 Dodecane liquid–vapour shock tube problem. Pressure, mixture velocity, mixture density and vapour dodecane
 495 mass fraction fields at $473\mu\text{s}$ after the initial contact discontinuity was removed. Comparisons between the exact solution
 496 and the numerical solutions of (Saurel, Petitpas and Abgrall, 2008) and the two-fluid model with different mesh resolutions.

497 3.2. Rising Bubble

498 The effective coupling between the two-fluid model and the implemented sharp interface method is
 499 evaluated against the behaviour of a rising bubble in a quiescent viscous liquid under the influence of
 500 the gravitational force. The dynamic deformation of a single rising bubble in a liquid column has been
 501 extensively examined with experimental studies (see selectively (Clift, Grace and Weber, 2005),
 502 (Bhaga and Weber, 1981), (Tomiya *et al.*, 2002) among many others). Thus, the obtained bubble
 503 shape diagram, also known as the Grace diagram (Clift, Grace and Weber, 2005), depicts
 504 comprehensively a regime classification based on the final bubble shape and its terminal velocity as a
 505 function of dimensionless numbers. From a numerical perspective, a rising bubble simulation is
 506 commonly used to validate interfacial flow solvers, due to the high variety of interface deformation
 507 patterns under slightly modified flow conditions. For this purpose, in the absence of any analytical
 508 solution, (Hysing *et al.*, 2009) performed a two-dimensional numerical benchmark configuration with
 509 different codes and established a reference solution for two numerical cases of different density and
 510 viscosity ratios between the gas bubble and the surrounding liquid. A numerical benchmark case of an
 511 initially circular gas bubble rising in an initially stagnant liquid with liquid density 1000kg/m^3 , liquid
 512 dynamic viscosity 10Pas and both density and viscosity ratios equal to 10, as proposed by (Hysing *et al.*,
 513 2009) is used here for validation of the developed method. The gravity in the system is $g=-0.98\text{m/s}^2$
 514 and the surface tension between the two fluids is $\sigma=24.5\text{N/m}$. Under these conditions, which
 515 correspond to intermediate Reynolds and Eotvos numbers with values 35 and 10, respectively, a
 516 moderate shape deformation is expected with a final bubble unbroken ellipsoidal shape based on the
 517 Grace diagram (Clift, Grace and Weber, 2005). The two-dimensional simulation was conducted with

518 the initial configuration and boundary conditions of Figure 3 in a uniform computational mesh of
 519 320×640 cells.



520

521 Figure 3 Initial configuration and boundary conditions for a two-dimensional circular gas bubble rising in a liquid column.

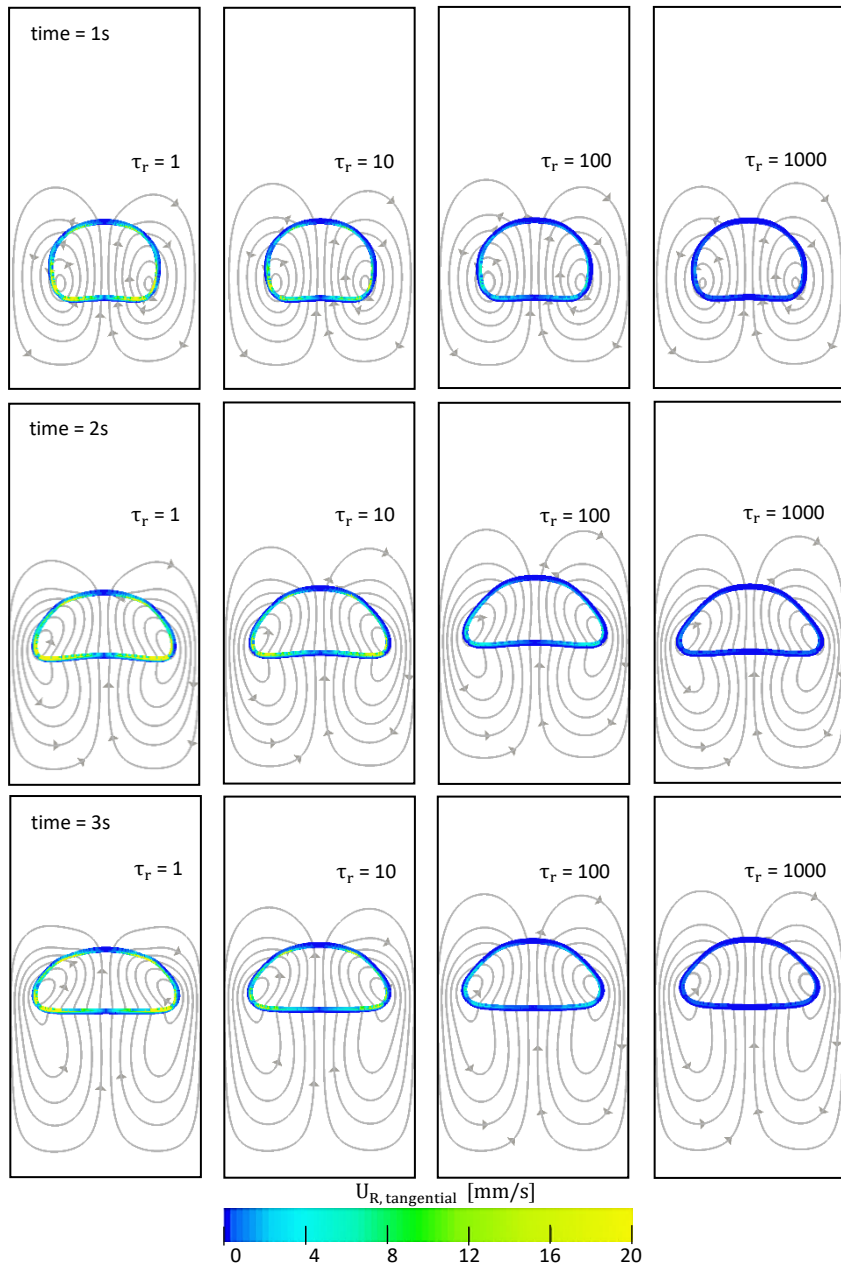
522 The rising bubble shape is presented in Figure 4 in three successive time instances and under the effect
 523 of different relaxation factor τ_r values, which appears in the artificial drag force of equation (8) as a
 524 case-dependent parameter to regulate an efficient coupling between the two-fluid model and the
 525 sharp interface approach. Focusing on the macroscopic evolution of the two-dimensional bubble
 526 interface, it is observed that the circular bubble is gradually deformed to an ellipsoid shape, due to
 527 the counter-action of gravitational and surface tension forces. Under the occurring ellipsoid regime
 528 (Clift, Grace and Weber, 2005), surface tension is dominant and mainly responsible for the evolution
 529 of a moderate bubble deformation without breakup of the interface. As it is also depicted in Figure 4,
 530 a stronger coupling between the two-fluid model and the sharp interface approach is achieved by
 531 maximizing the relaxation factor, corresponding to the elimination of the interfacial relative velocity.
 532 This numerical trick practically overcomes the two-fluid principle of the mathematical model, which
 533 imposes different velocity fields for each phase and approaches a standard sharp interface
 534 formulation, in which the two phases share a single momentum equation and respect the no-slip
 535 condition on the interface. Additionally, an increase of the relaxation factor, apart from the gradual
 536 elimination of the gas liquid relative velocity on the interface, has an apparent effect on the
 537 macroscopic bubble shape development.

538 However, the case-dependent calibration of τ_r has been avoided with the implementation of an on-
 539 the-fly algorithm which evaluates the interfacial region and gradually increases the value of τ_r , until
 540 the point that the tangential component of the relative velocity on the interface reaches a defined
 541 lower-bound close to zero. More specifically, in each iteration of the pressure correction the
 542 computational cells in the interfacial regions are evaluated to meet the no-slip condition. The criterion
 543 used relates the tangential component of the relative velocity on the interface with its total local value
 544 and sets a sufficiently low lower-bound, as follows:

545
$$|u_{r,tangential}| < 10^{-5}|u_r|$$

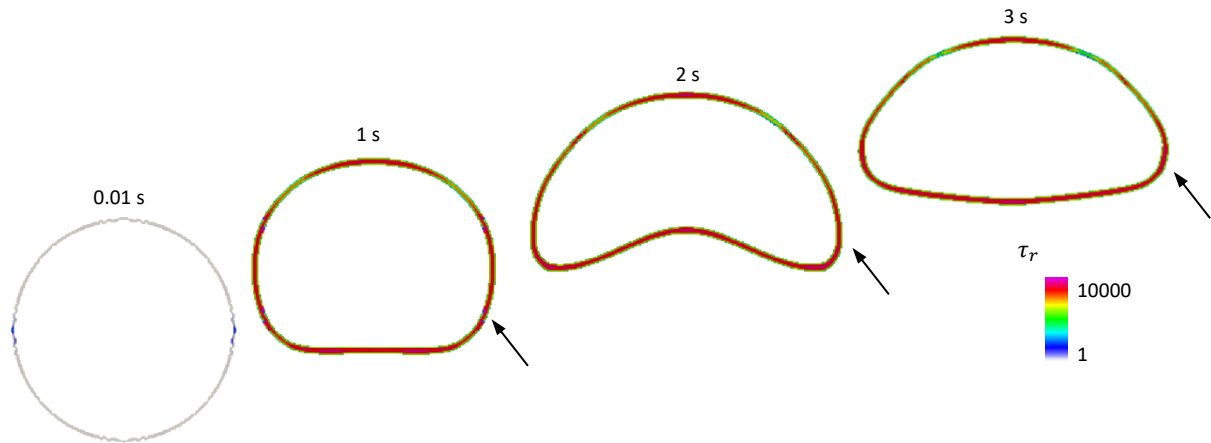
546 In the case that the above condition is not satisfied, the τ_r value is increased starting from the value of
 547 1 for each interfacial cell in each new time step of the pressure correction algorithm. In order to avoid
 548 significant jumps on the drag force values and to improve the performance with reduction of the
 549 computation cost, a smoothing of the τ_r values in the neighbour cells is performed. A demonstration
 550 of the algorithm with different local values for τ_r with respect to the no-slip interface condition is
 551 illustrated in Figure 5 for the rising bubble. The maximum values for τ_r are observed on the sides of

552 the rising bubble, where also peaks in the relative velocity are observed due to the vertical motion of
553 the bubble in the surrounding liquid.



554

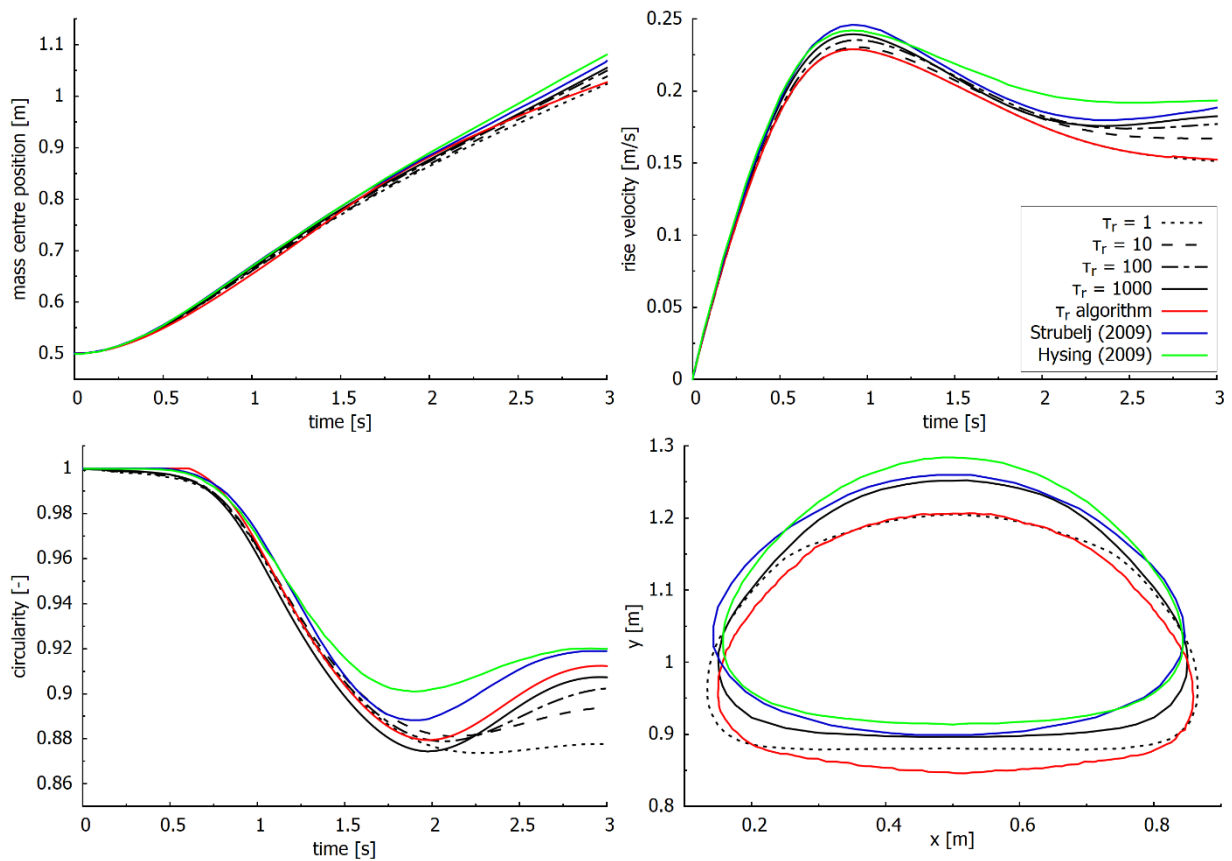
555 Figure 4 Tangential relative velocity distribution on the interface of a rising bubble and gas liquid mixture velocity vectors at
556 successive times under the effect of different relaxation factors τ_r .



557

558 Figure 5 Relaxation factors τ_r calculated on the interface of the rising bubble with the on-the-fly algorithm for meeting the
 559 no-slip interfacial condition.

560 In the scope of a rigorous quantitative analysis, the mass centre position, the mean rise velocity and
 561 the deformed bubble circularity obtained with different relaxation factor values are examined in
 562 Figure 6. The computed benchmark quantities are compared with the reference solution of (Hysing *et al.*,
 563 2009) and the results presented by (Štrubelj, Tiselj and Mavko, 2009), using a similar concept of
 564 coupling the two-fluid model with an interface sharpening approach; in this case, a conservative level
 565 set method has been utilised. Hereby, it is verified that a stronger coupling with the implementation
 566 of maximum value for the relaxation factor ensures that the evolution of the rising bubble will reach
 567 the expected behaviour. Specifically, the final position of the bubble centre of mass with the optimum
 568 relaxation factor $\tau_r=1000$ is at 1.055m and differs 1.22% from (Štrubelj, Tiselj and Mavko, 2009) results.
 569 Furthermore, the maximum rise velocity is observed at 0.92s and with a value of 0.239m/s deviates
 570 by 2.58% from (Štrubelj, Tiselj and Mavko, 2009) solution. Regarding the bubble shape deformation,
 571 the minimum circularity value occurs at 1.98s, approximately 0.1s later than in (Štrubelj, Tiselj and
 572 Mavko, 2009) study; however, with respect to the tendency of circularity evolution in time the
 573 quantitative error is 1.7%. Finally, the shape of the rising bubble at its final position at 3s, as calculated
 574 with both the minimum and maximum relaxation factor values, shows the significant effect of an
 575 effective coupling between the two-fluid model and the sharpened interface approach on the bubble
 576 shape development with regards to the results in the literature (Hysing *et al.*, 2009), (Štrubelj, Tiselj
 577 and Mavko, 2009). The results obtained from the on-the-fly algorithm also meet a satisfactory
 578 agreement with the reference solution and show that the use of the proposed automatic algorithm
 579 for calibrating on-the-fly the relaxation factor τ_r is a good compromise to avoid any arbitrary case-
 580 dependent calibration and the significantly increased computational cost, when the artificial drag
 581 force is maximised in the whole interfacial region with an effect on the converge of the pressure
 582 correction algorithm.



583

584 Figure 6 Bubble benchmark quantities, i.e. mass centre position, rise velocity and circularity, evolution in time under the effect of different relaxation factors τ_r . Bubble shape at its final position at 3s computed with minimum and maximum τ_r
 585 values. Comparisons with the reference solution of (Hysing *et al.*, 2009) and the simulation results performed by (Štrubelj, Tiselj and Mavko, 2009).
 586
 587

588 3.3. High-Speed Droplet Impact

589 3.3.1. Experimental Set-up

590 In order to validate the multiscale approach developed, new experiments have been performed for a
 591 droplet impact onto a solid surface. The experiments have been conducted at the University of
 592 Magdeburg and concern a water droplet impact onto a high-speed moving target in three different
 593 cases summarized in Table 2. The deionized water droplet is slightly deformed to an ellipsoid shape,
 594 due to the acoustic field which keeps it levitated; the droplet is hit by the flat and smooth moving
 595 target, propelled from an initial distance of 2.35m away from the levitating droplet. The experiments
 596 were performed at room temperature 21°C and atmospheric pressure conditions; the surface tension
 597 between the water droplet and the surrounding air is equal to 0.072N/m. The high-speed impact
 598 velocities of 120, 150 and 200m/s correspond to significantly high Weber and Reynolds numbers both
 599 of the order of 10^5 to 10^6 , as calculated for the droplet properties at impact conditions. The rapid
 600 droplet splashing and the subsequent violent fragmentation of the produced secondary structures
 601 were visualized with the use of a high speed camera of 5 million frames per second and a spatial
 602 resolution of 50 μ m per pixel; recording of video started when the moving target was approximately
 603 3.17mm away from the droplet.

604

605

606

607 Table 2 Impact conditions for the examined experimental cases of high-speed droplet impact on a moving target.

case	d_x [mm]	d_y [mm]	u_{imp} [m/s]	target	We [-]	Re [-]	Oh [-]
1	2.017	1.55	120	teflon	3.6×10^5	2.2×10^5	7.6×10^{-3}
2	2.65	2.2	150	teflon	7.6×10^5	3.7×10^5	5.5×10^{-3}
3	2.14	1.796	200	acrylic	1.1×10^6	4.2×10^6	6.9×10^{-3}

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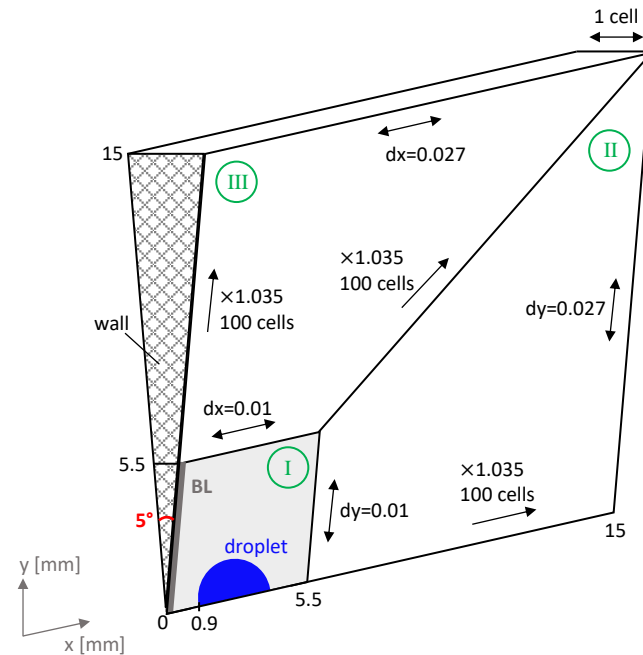
609 3.3.2. Simulation Results

610 For the numerical simulations of high-speed droplet fragmentation, the problem is set-up in a different
611 but corresponding manner with the water droplet moving with the impact velocity towards a rigid
612 wall target. The simulations were performed in a 3D wedge geometry with one cell thickness, using a
613 computational mesh of 412,500 cells; the details are described in Figure 7. For the purpose of a grid
614 dependency investigation regarding the multiscale model functionality, two additional computational
615 meshes have been used with twice coarser and twice finer resolution compared to the original mesh
616 in the region around the droplet and wall interaction, illustrated as zone I in Figure 7. At the initial
617 time step the moving droplet is set 0.9mm away from the rigid wall. Apart from the liquid phase
618 velocity field, which is initialized with the initial velocity of the moving droplet, the air velocity field is
619 also initialized from a developed field obtained with the impact velocity set as an inlet in the right
620 patch of the computational domain. Using this configuration, the effect of the moving target on the
621 surrounding air in the original experimental set-up is adequately represented in the conducted
622 simulations. The liquid gas interface surface area density is initialized on the droplet interface as the
623 surface area of an ellipsoid with the dimensions of the examined water droplet which corresponds to
624 a 5° wedge per unit of the local computational cell volume. On the wall, the no-slip boundary condition
625 is applied for the velocity fields, while a Neumann boundary condition is satisfied for the other
626 computed flow fields.

627 The spatial discretization used is based on second order linear discretization schemes, limited towards
628 a bounded first order upwind scheme in regions of rapidly changing gradients. Time stepping is
629 performed adaptively during the simulation, so as to respect the selected limit for the convective
630 Courant–Friedrichs–Lewy (CFL) condition of 0.4. Even though the turbulent state corresponds to fully
631 3D-developed phenomena, the evolution of the droplet fragmentation under the examined impact
632 conditions is found to be significantly quicker compared to the turbulence time scales. Therefore, the
633 configuration of Figure 7, which is utilised in the performed simulations, is an acceptable compromise
634 between the accuracy of the numerical model and a viable computational cost.

635 The simulations conducted were based on the assumption that the liquid phase is the only present
636 dispersed phase, interpenetrating and interacting with the continuous air phase. Under the high-
637 speed impact conditions corresponding to very high Weber numbers ranging from 10^5 to 10^6 , the
638 droplet impact on the wall and the imposed prompt splashing will evolve rapidly; thus, contact angle
639 boundary conditions are not explicitly defined and a zero gradient boundary condition for the water
640 volume fraction on the wall is imposed (Kyriazis, Koukouvinis and Gavaises, 2018). With regards to
641 phase-change phenomena, vaporisation plays a minor role at the early stages of impact, since the
642 temperature variations around the room conditions are not significant in comparison to the other
643 physical phenomena that take place (Kyriazis, Koukouvinis and Gavaises, 2018). Specifically, in the
644 present simulations the local water temperature does not increase more than 20K at the moment of
645 impact, when the strong shock wave is formed inside the droplet and the maximum local pressure of
646 about 10^8 Pa is observed. On the contrary, cavitation is produced inside the droplet due to the
647 influence of strong compressibility effects; however, in this particular case its influence is negligible

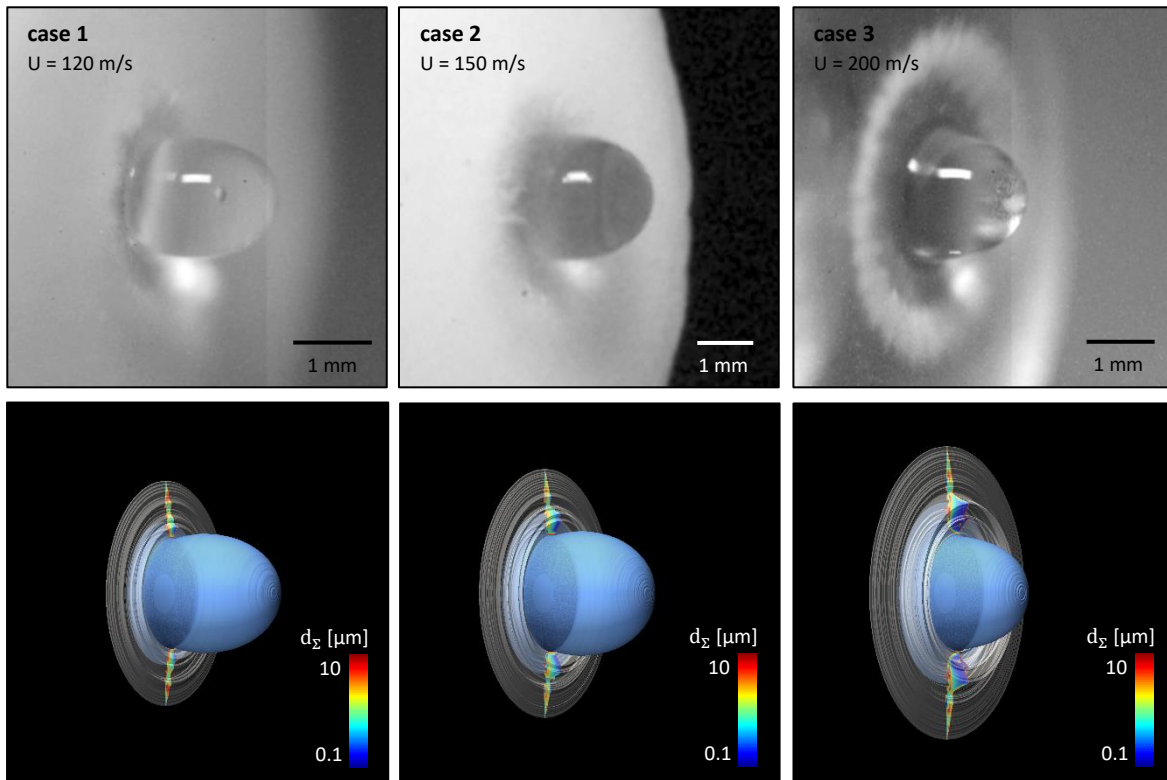
648 compared to other dominant physical phenomena and it is not taken into consideration in the
 649 numerical modelling, as it is analysed in detail in the following paragraphs.



650

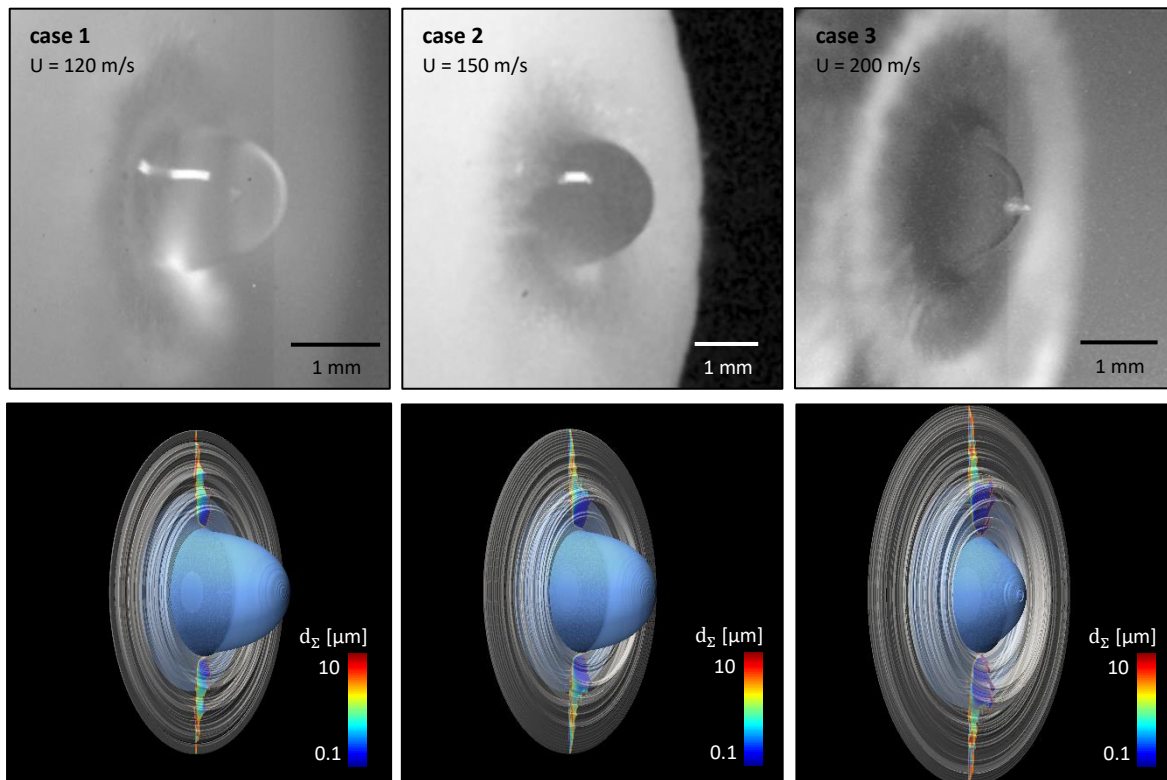
651 Figure 7 Initial configuration and information regarding the computational mesh for the simulation of high-speed droplet
 652 impact on a rigid wall.

653 The evolution of the droplet fragmentation at 2, 4 and 6 μ s after the impact on the target are presented
 654 in Figures 8, 9 and 10, respectively, as it has been captured by the experimental study and the
 655 performed simulations with the proposed multiscale two-fluid model under the three different impact
 656 conditions of Table 2. In the numerical investigation, the widespread and highly dispersed water cloud
 657 produced after the prompt splashing of the droplet is subject to the diffuse interface formulation of
 658 the multiscale two-fluid model, shown as a grey iso-surface in the results. Therefore, the dominant
 659 sub-grid scale structures are modelled accordingly within the dispersed flow regime formulation of
 660 the numerical model and the interface surface area density diameters are calculated and used in the
 661 drag force calculations. Despite the vast spectrum of scales involved, the macroscopic characteristics
 662 of the successive stages of the droplet fragmentation are adequately predicted by the performed
 663 simulations, with the corresponding results to depict the radially expanding water cloud. In cases 1
 664 and 2, which correspond to Weber numbers at impact conditions of the order of 10^5 , a similar
 665 evolution of the phenomenon is observed with an expected more rapid water dispersion under the
 666 impact velocity of 150m/s. On the contrary, in case 3 the increase in the Weber number of the order
 667 of 10^6 results to a significantly violent droplet splashing with a widespread water cloud corona to be
 668 captured both by the experimental results and the simulation. However, the water microjet injected
 669 from the centre of the deforming droplet surface opposite to the droplet motion, which is depicted in
 670 the experimental captures as an effect of the secondary cavitation formation inside the droplet, is a
 671 low intensity phenomenon compared to the dominant and rapid water dispersion.



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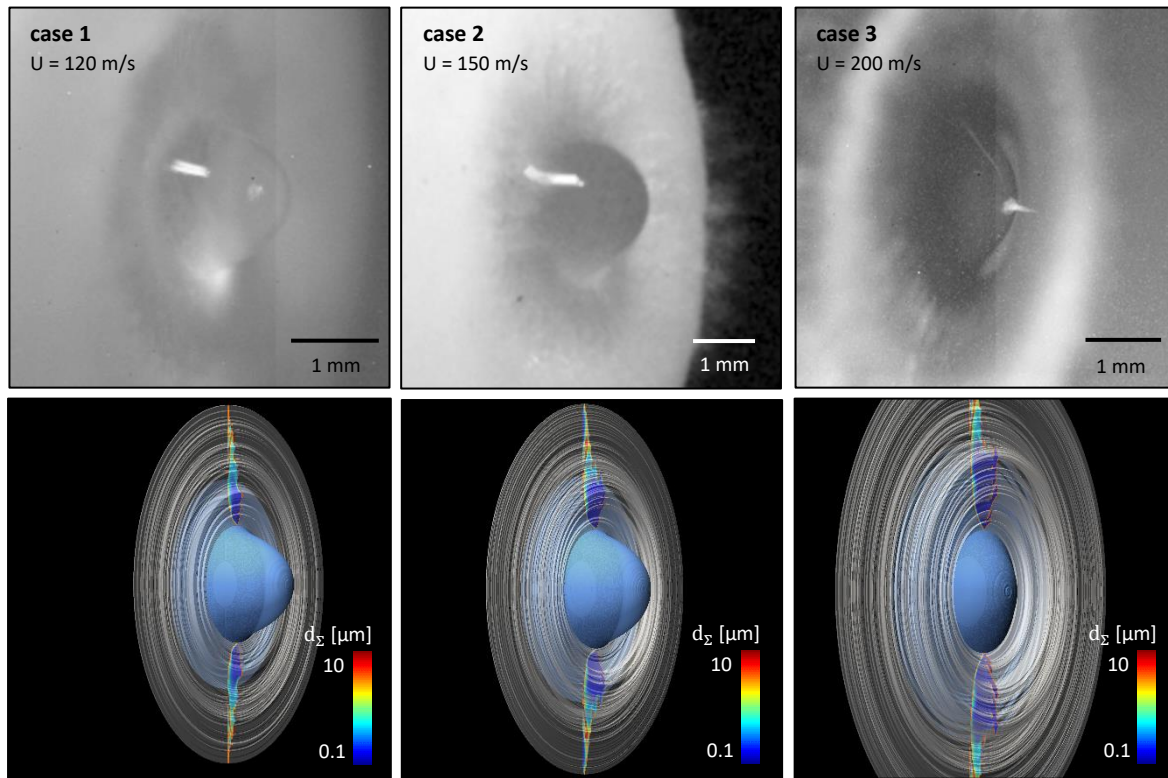
673 Figure 8 Droplet fragmentation $2\mu\text{s}$ after impact on the target in cases 1, 2, 3. Comparison between the experimental results
 674 captured 32° from the perpendicular view and the 3D reconstructed flow fields from the simulation. Blue iso-surface
 675 represents the sharp interface regions and grey iso-surface the diffuse interface regions calculated with the multiscale two-
 676 fluid approach.



677

678 Figure 9 Droplet fragmentation $4\mu\text{s}$ after impact on the target in cases 1, 2, 3. Comparison between the experimental results
 679 captured 32° from the perpendicular view and the 3D reconstructed flow fields from the simulation. Blue iso-surface

680 represents the sharp interface regions and grey iso-surface the diffuse interface regions calculated with the multiscale two-
 681 fluid approach.



682
 683 Figure 10 Droplet fragmentation $6\mu\text{s}$ after impact on the target in cases 1, 2, 3. Comparison between the experimental results
 684 captured 32° from the perpendicular view and the 3D reconstructed flow fields from the simulation. Blue iso-surface
 685 represents the sharp interface regions and grey iso-surface the diffuse interface regions calculated with the multiscale two-
 686 fluid approach.

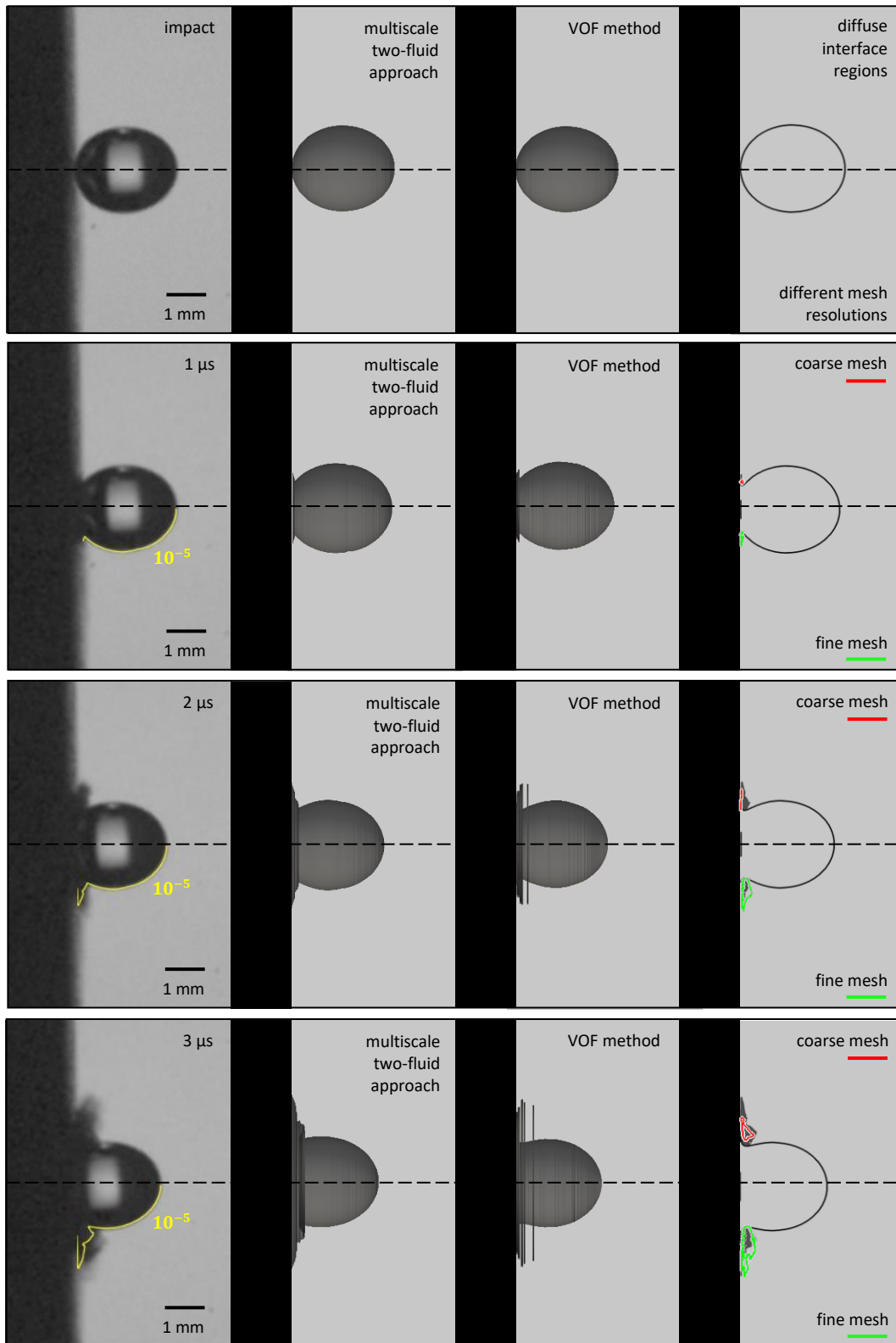
687 The evolution of the droplet impact with the target under the impact velocity of 150m/s (case 2), the
 688 prompt splashing at the early stages of impact along with the severe fragmentation and water
 689 dispersion at later stages are presented in Figures 11 and 12. In successive time instances, the
 690 experimental video snapshots are compared with the 3D reconstructed water volume fraction iso-
 691 surface at 10^{-3} obtained from the performed simulations with the proposed multiscale two-fluid model
 692 and the compressibleInterFoam solver, which is based on a VOF method commonly used for this type
 693 of problems. The iso-line of the water volume fraction at a value of 10^{-5} , as calculated with the
 694 multiscale two-fluid approach, is plotted against the experimental results. Moreover, the detected
 695 dispersed flow regions using 3 different computational grids, namely the original grid of Figure 7 along
 696 with two new grids with twice coarser and twice finer resolution in region I, respectively, are
 697 presented to depict the dependency of the interfacial approaches capabilities and the performed
 698 topological investigation on the local mesh resolution.

699 As it can be observed in Figure 11, at the moment of impact the flow field is dominated by a segregated
 700 flow regime with perfectly separated two phases as defined by the droplet interface. Thus, up to this
 701 point, the sharp interface approach is applied exclusively in the whole flow field; good results are
 702 obtained with respect to the initial droplet shape. At that time, the occurring impact conditions
 703 correspond to a very high Weber number of 7.6×10^5 and thus, a prompt splashing is imposed driven
 704 by the dominant droplet inertia. Subsequently, the violent impact conditions do not allow for a liquid
 705 lamella to be formed, as depicted in the experimental results; instead, the production of a dense cloud
 706 of secondary droplets and ligaments is observed, which is moving radially ahead of the deformed

707 droplet. At these stages, which correspond to times 1-3 μ s in Figure 11, the topological algorithm
708 detects the first transitions in the dispersed flow regime; the cloud of the produced fluid structures
709 after the droplet and wall impact is subject to a diffuse interface approach, since it consists of
710 structures smaller than 10⁻⁵m that cannot be resolved by the local mesh resolution. On the contrary,
711 the simulation with the VOF method applied in the whole flow field captures accurately the tendency
712 of a radial water expansion. However, the overall sharp interface formulation leads to the prediction
713 of an unphysical thin water film after the impact, as in the case of a well-formed lamella under
714 moderate impact conditions, instead of the experimentally observed wide cloud of secondary
715 droplets. This predicted behaviour corresponds to the deficiency of the VOF method to resolve small
716 fluid structures in the sub-grid scale limit. As a result, the computational cells with relatively small
717 volume fractions, that imply the existence of microscale secondary droplets, are underestimated and
718 therefore, a thin water film is calculated in the regions of a high water volume fraction concentration.
719 It is interesting to notice that at the examined early stages of impact, the multiscale two-fluid model
720 with a finer mesh can predict more accurately the extent of the water spatial dispersion compared to
721 the original or an even coarser mesh, as it is illustrated in Figure 11 at 2 and 3 μ s. Given the fact that
722 large-scale structures dominate the dispersed regions at the first time instances after impact, it is
723 expected that a finer mesh can obtain most of the flow field information with the multiscale model to
724 operate under a diffuse interface approach. Nevertheless, this is not the case for the later stages of
725 impact, in which the microscale droplets overtake the larger initially produced droplets of the dense
726 water cloud, as it will be discussed afterwards.

727 Later stages of the droplet impact are depicted in Figure 12, where the flow is highly dispersed with
728 an extended cloud of secondary features expanding radially away from the target. A widespread
729 dispersed region in the form of an expanding corona is also captured by the multiscale two-fluid
730 model; however, the calculated radial water dispersion is limited compared to the experimental
731 observation. More specifically, after 4 μ s in regions of apparent water concentration in the experiment,
732 approximately 1 mm away from the target, there is not any significant amount of water volume
733 fraction present in the simulation. Moreover, as shown in Figures 8, 9, 10, the smaller structures are
734 underestimated at the outer sides of the expanding cloud and the mixing of the injected water with
735 the surrounding air is limited. Due to the supersonic conditions of the expelled surrounding air at the
736 later stages of impact and the significant increase in local air temperature, vaporisation may be the
737 key mechanism of water dispersion at the borders of the expanding water cloud; thus, the
738 consideration of vaporisation effects should lead to an improved and more realistic capturing of the
739 extended water dispersion at the later stages of impact. However, as it is comprehensively presented
740 in Figure 13, the vertical expansion of both the attached on wall water film and the dispersed
741 secondary droplets cloud is well predicted with the performed simulation under the existing highly
742 multiscale conditions in the course of the impact and meets satisfactorily the experimental
743 measurements for the lower values of the water volume fraction. Therefore, the obtained results
744 provide a relatively accurate insight into the presence of an extended and chaotic water dispersion in
745 contrast to the VOF method results, which are restricted to a non-realistic water film spreading with
746 only a few droplets being formed as a numerical result of the strict sharp interface implementation.
747 Within the scope of a grid dependency analysis, it is noticeable in Figure 12 that for the occurring
748 dominant dispersed flow regime, a coarser computational mesh along with the multiscale approach
749 can provide locally a more extended radial water dispersion region. Some of the original
750 computational cells with negligible water volume fraction are now incorporated to neighbour cells
751 and therefore, are subject to a diffuse interface regime for the modelling of local sub-grid scale
752 secondary droplets with dimensions even less than 1 μ m. This behaviour comes in contrast to the
753 results obtained with the multiscale approach and a finer mesh, which predict a limited radial water

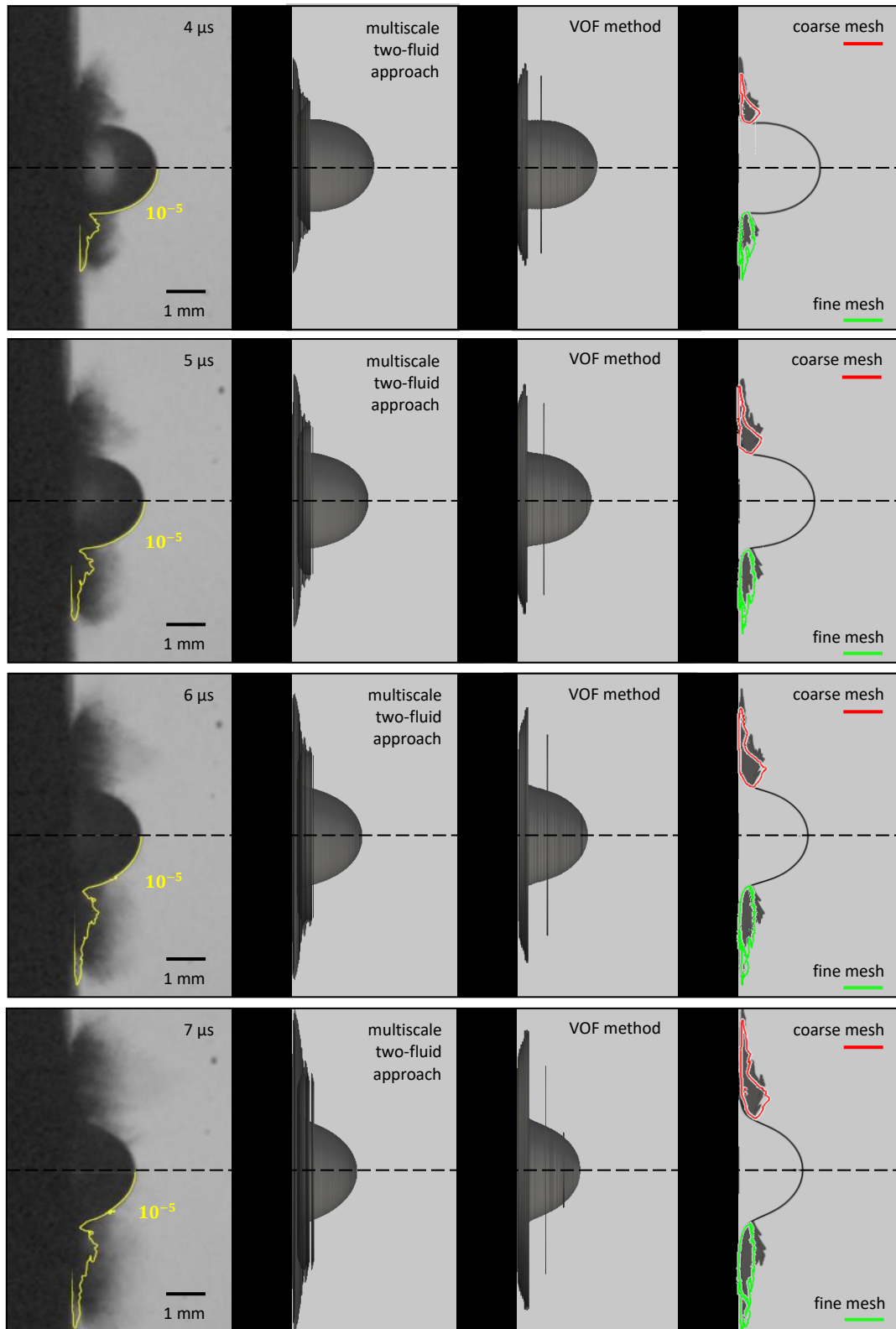
754 spreading and approach the results of the pure VOF simulation. Consequently, the application of the
755 multiscale two-fluid model in flow regions with multiple dynamic transitions between the segregated
756 and dispersed regimes using a locally uniform computational grid, as performed in the conducted
757 simulations, requires a compromise regarding the selected grid resolution. More specifically, given the
758 numerical limitations of the VOF and the diffuse interface methods with respect to the computational
759 grid and the switching criteria of the flow topology detection algorithm, an intermediate grid
760 resolution is defined as optimum.



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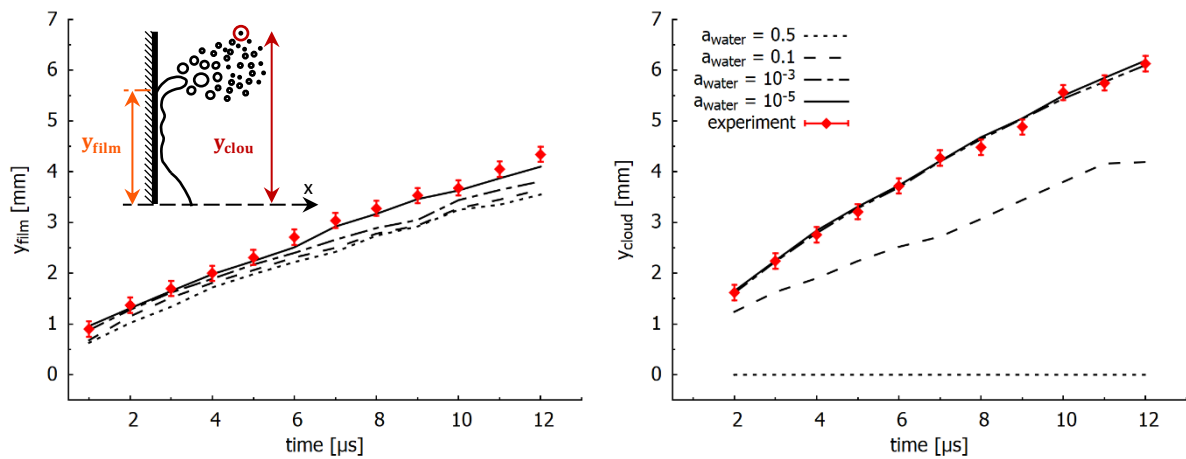
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Figure 11 Early stages of droplet impact with the target under the impact velocity of 150m/s (case 2). Comparisons between the experimental results from side view and the 3D reconstructed water volume fraction iso-surface at 10^{-3} obtained with the multiscale two-fluid model and the VOF method. The diffuse interface regions, calculated with the multiscale two-fluid model using 3 different mesh resolutions, are compared in the last column. Yellow iso-line represents the water volume fraction at 10^{-5} , red isoline the diffuse interface regions using a coarse mesh and green isoline the diffuse interface region using a fine mesh.



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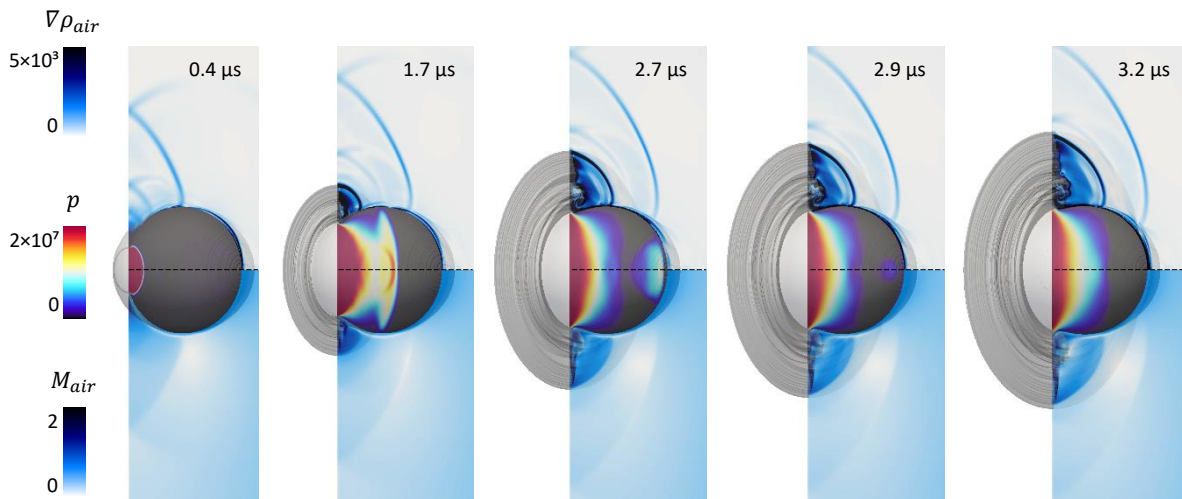
769 Figure 12 Later stages of droplet impact with the target and intense water dispersion under the impact velocity of 150m/s
 770 (case 2). Comparisons between the experimental results from side view and the 3D reconstructed water volume fraction iso-
 771 surface at 10^{-3} obtained with the multiscale two-fluid model and the VOF method. The diffuse interface regions, calculated
 772 with the multiscale two-fluid model using 3 different mesh resolutions, are compared in the last column. Yellow iso-line
 773 represents the water volume fraction at 10^{-5} , red isoline the diffuse interface regions using a coarse mesh and green isoline
 774 the diffuse interface region using a fine mesh.



775

776 Figure 13 Droplet fragmentation under the impact velocity of 150m/s (case 2). Comparisons between the experimental and
 777 the numerical results with different water volume fraction values for the vertical expansion of the attached on wall water
 778 film and the secondary droplets cloud.

779 The high-speed droplet impact is governed by significant compressibility effects inside the droplet at
 780 the early stages of the interaction with the rigid wall. After the moment that the droplet reaches the
 781 wall, a strong shock wave is formed inside the droplet with local pressure up to 1200bar, as depicted
 782 in Figure 14 at $0.4\mu\text{s}$. The shock wave is propagating and moving outwards, opposite to the droplet
 783 motion, while it gradually overtakes the contact line between the target and the deforming droplet.
 784 At $1.7\mu\text{s}$ it is observed that the shock wave is reflected normal to the droplet outer free surface and
 785 an expansion wave adjacent to the free surface is created (Haller *et al.*, 2002), (Wu, Xiang and Wang,
 786 2018). Afterwards, the shock wave propagation continues with the formation of an increasing low
 787 pressure region inside the droplet, until the time it reaches the boundary of the deforming droplet
 788 interface and it is reflected backwards at $2.7\mu\text{s}$. This shock wave reflection results to the creation of
 789 strong rarefaction waves (Haller *et al.*, 2002), (Wu, Xiang and Wang, 2018) at $2.9\mu\text{s}$, which could result
 790 to extended cavitation regions inside the droplet. However, it has been shown in previous numerical
 791 studies (Niu and Wang, 2016), (Kyriazis, Koukouvinis and Gavaises, 2018), (Wu, Xiang and Wang, 2018)
 792 that under similar conditions the produced vapour volume fraction after the shock wave reflection
 793 does not exceed the value of 0.03, defining a non-significant cavitation effect. Since the droplet impact
 794 evolution is not driven by cavitation under the examined impact conditions, a model for cavitation has
 795 not been implemented in the developed multiscale framework; instead, a very small volume fraction
 796 of air of order of 10^{-6} , which corresponds to the nucleation volume fraction, is introduced in the initial
 797 droplet volume fraction. Under this assumption, the small gaseous volumes inside the droplet will
 798 expand after the significant pressure drop, leading to volumes equal to those that would occur with
 799 cavitation. The pressure evolution inside the droplet will continue with the gradual elimination of the
 800 created regions of small gaseous volumes, as long as the droplet widespread splashing is dominating
 801 the surrounding flow field.

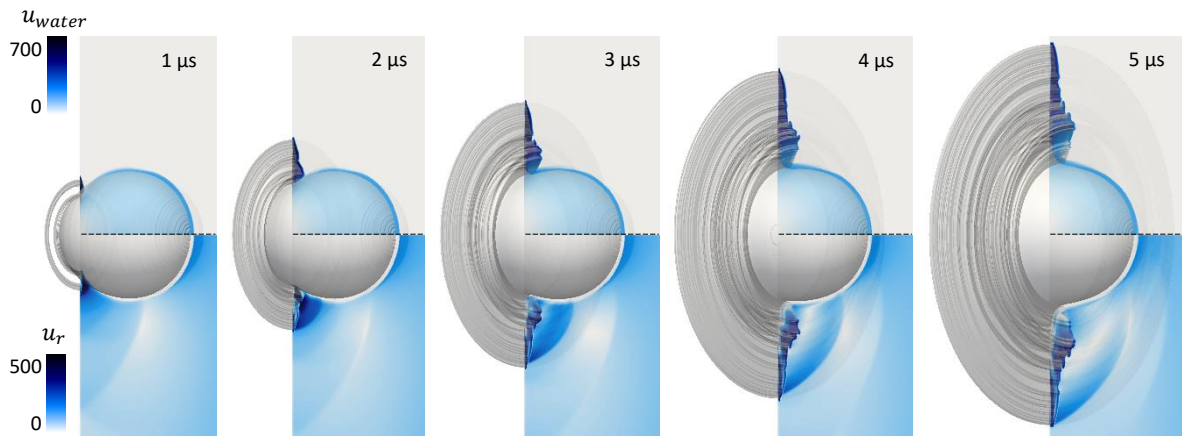


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803 Figure 14 Time evolution of the pressure field inside the droplet, the shock wave formation and propagation along with the
 804 density gradient and the Mach number for the surrounding air after the droplet impacting the rigid target with a velocity of
 805 150m/s (case 2).

806 After the droplet impact and along with the beginning of a strong shock wave propagation inside the
 807 droplet, the development of a high speed jetting is observed in Figure 15. The injected water film,
 808 which just after the droplet impact at 1μs has a velocity 5 times larger than the impact velocity, is
 809 responsible for the rapid lateral and radial water dispersion. This observation also meets the
 810 experimental measurements of a maximum liquid film expanding velocity at around 720m/s. At the
 811 same time, a supersonic flow with strong propagating shock waves is observed in the surrounding air,
 812 due to the high speed dispersion of the produced water cloud. As illustrated in Figure 14, the
 813 formation and high-speed injection of the water film at the early stages of the droplet impact,
 814 corresponds to a violent displacement of the surrounding air, resulting to a supersonic flow for the air
 815 with local Mach numbers up to 2.5. Subsequently, during the droplet lateral spreading on the wall
 816 target, the intensity of the initial jetting and the propagating shock waves in the air is reduced;
 817 however, the velocities of the water phase remain significant with peaks on the dispersed flow regions
 818 where the secondary droplets cloud is penetrating the surrounding air. An examination of the
 819 temporal and spatial evolution of the relative velocities between the droplet and the surrounding air
 820 in Figure 15 comes to the same conclusion that the highest water velocities occur at the borders of
 821 the expanding water cloud. Thus, in highly dispersed flow regions, where practically very small
 822 droplets are present, the consideration of aerodynamic and slip velocity effects increases the physical
 823 coherency of the numerical model.

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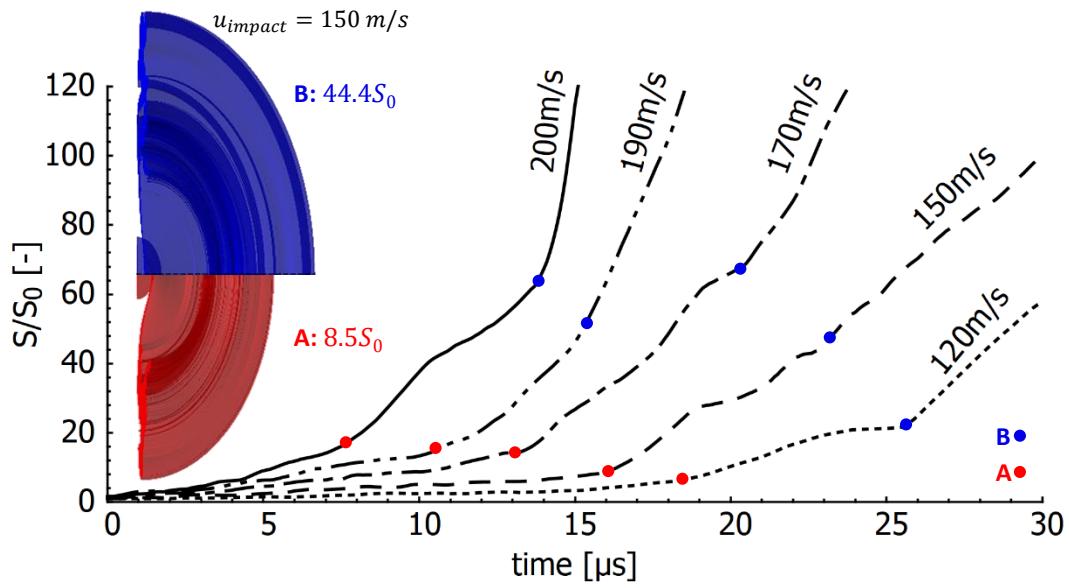


825

826 Figure 15 Time evolution of the water velocity field inside the droplet and the relative velocity field in the surrounding area
827 after the droplet impacting the rigid target with a velocity of 150m/s (case 2).

828 In Figure 16 the temporal evolution of the calculated interface surface area under different impact
829 velocities is presented, as it is obtained from the transport equation for the liquid gas interface surface
830 area density (5). A similar pattern regarding the interface surface area production over time is
831 observed irrespectively of the impact conditions. More specifically, after the droplet impact the
832 interface surface area is gradually increasing with the same rate till approximately point A. These time
833 instances, as shown in Figure 17, correspond to the early stages of splashing, where the water film
834 lateral spreading on the wall target dominates the formation and expansion of the dispersed water
835 cloud. Since the surface area of the undeformed droplet interface remains unchanged, the maximum
836 values of the interface surface area are observed on the dispersed regions away from the wall target
837 where sub-grid scale turbulent mixing and secondary droplet coalescence and breakup have a crucial
838 effect on interface production, as described in equation (5). After that and until approximately point
839 B in Figure 16, the interface surface area performs a rapid increase which is more intense with an
840 increase on the impact velocity and is related to later stages of the fragmentation evolution with the
841 water dispersion becoming the main effect on interface production. After point B and until the end of
842 the observation of the phenomenon, an almost smooth increase in interface surface area is shown
843 due to the penetration of the already produced secondary droplets cloud in the surrounding area.

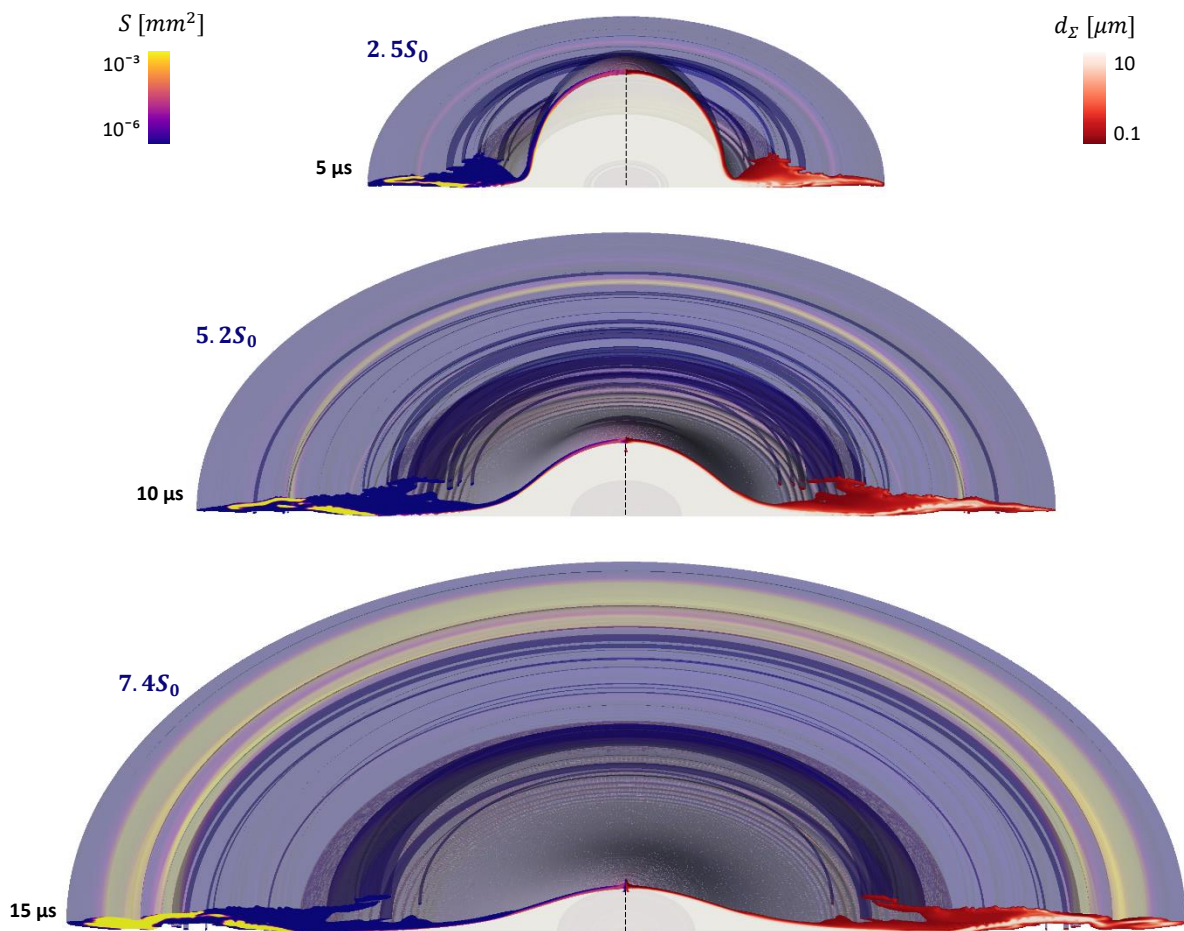
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846 Figure 16 Time evolution of the interface surface area for the developed water cloud and the secondary flow features after
 847 the droplet impact on wall with respect to the initial ellipsoid droplet surface area S_0 under different impact velocities. As
 848 time zero is set the moment of impact onto the rigid wall for the droplet with impact velocity 150m/s.

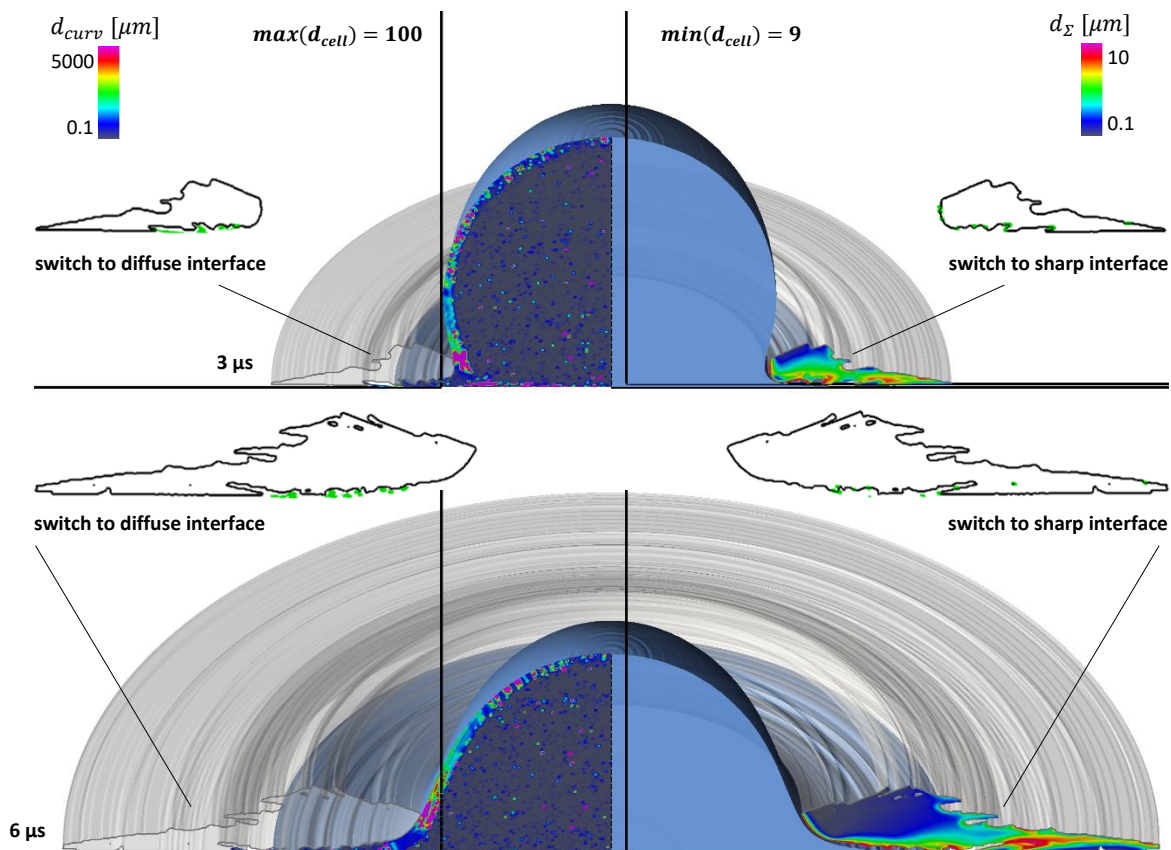
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851 Figure 17 Characteristic instances of the interface surface area evolution with respect to the initial ellipsoid droplet surface
 852 area S_0 and the calculated interface surface area density diameters under the impact velocity of 150m/s (case 2).

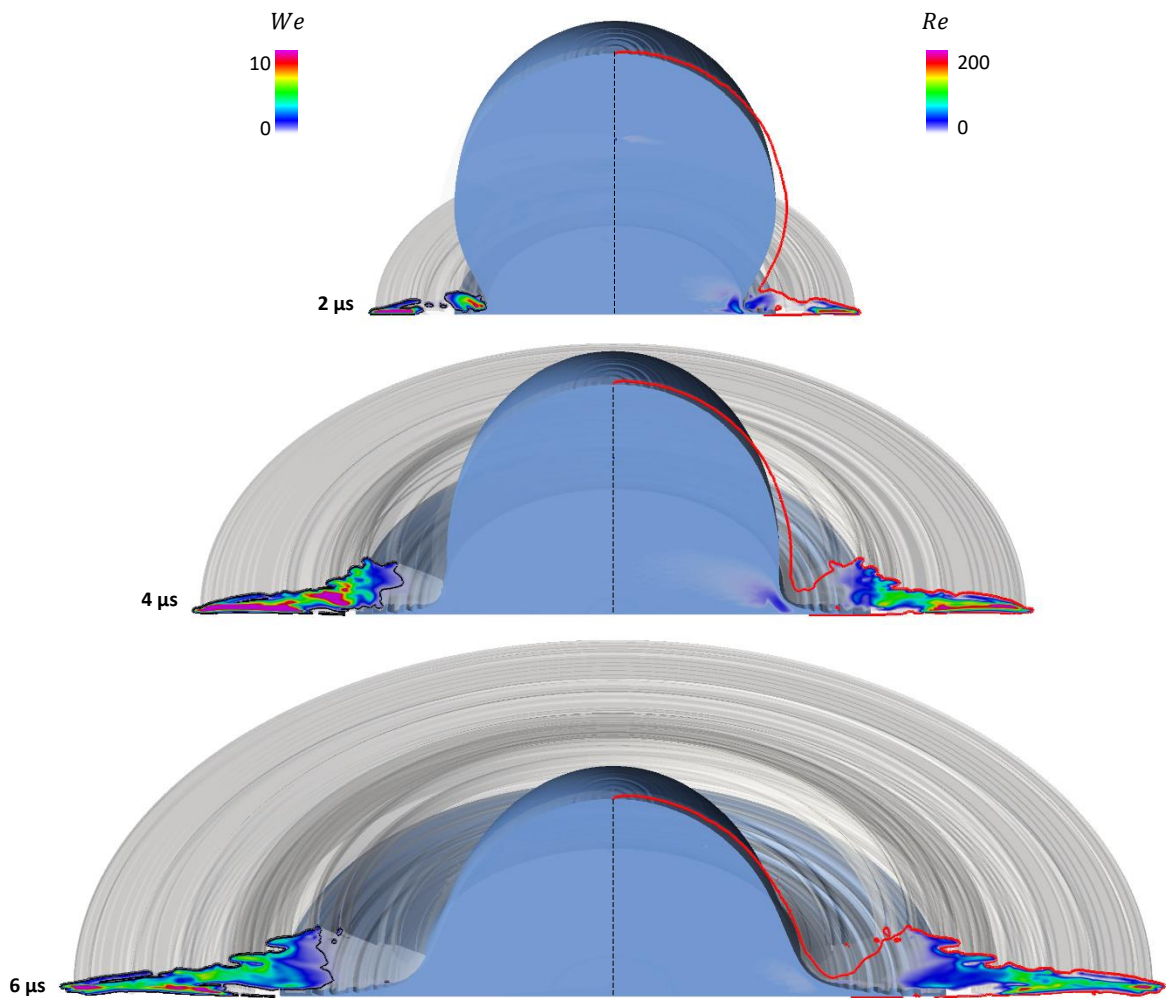
853 In Figure 18, two characteristic time instances at the earlier and later stages of the droplet
854 fragmentation under the impact velocity of 150m/s are selected to depict the functionality of the flow
855 topology detection algorithm. On the left side of the axis of symmetry are illustrated the calculated
856 diameters based on the interface curvature d_{curv} , which are used for the first geometric criterion of
857 equation (16) in the sharp interface regions. As shown, the local interface curvature can obtain
858 relatively large values which based on equation (15) are correlated with small fluid structures,
859 reaching the limit of the local mesh resolution and the accuracy capabilities of the sharp interface
860 approach. However, only the geometric criterion is not sufficient to keep a physical consistency
861 regarding the areas of small d_{curv} values, with such small fluid structures to be detected even in areas
862 inside the deforming droplet core where the presence of small droplets has no physical interpretation.
863 Thus, the additional topological criteria are the key factor in introducing a switching between sharp
864 and diffuse interface approaches with respect to the local flow development and the physical
865 transition from a segregated to a dispersed flow regime. The computational cells which satisfy both
866 the geometric and the topological criteria and are subject to a diffuse interface formulation in the
867 following time step are marked in green. As expected, these regions are detected at the borders of
868 the already diffuse interface regions within the dispersed water cloud and they concern relatively large
869 flow structures, which were previously resolvable by the mesh resolution with local minimum cell sizes
870 of 10^{-5} m. On the right side of figure 18 the calculated interface surface area density diameters d_{Σ} for
871 the currently diffuse interface region within the highly dispersed secondary droplet cloud are
872 illustrated. As shown, the local diameters used for the local drag force calculation range from the
873 spectrum of microscales to 10^{-5} m, which is the local minimum cell size and correspondingly the limit
874 for a sub-grid scale analysis. In both time instances there are detected a few computational cells in
875 the borders between sharp and diffuse interface approach regions with d_{Σ} that exceed the local cell
876 dimensions; these computational cells are subject to a sharp interface approach based on the
877 geometric criterion of equation (17).



878

879 Figure 18 Droplet fragmentation with impact velocity 150m/s (case 2). Blue iso-surface represents the sharp interface regions
 880 and grey iso-surface the diffuse interface regions calculated with the multiscale two-fluid approach. (on the left) The
 881 calculated diameters based on the interface curvature. In green are marked the cells switching from sharp to diffuse interface
 882 approach. (on the right) The calculated interface surface area density diameters. In green are marked the cells switching
 883 from diffuse to sharp interface approach.

884 Considerable emphasis has been put on correlating the geometric switching criteria of the flow
 885 topology detection algorithm, which in essence act as an indication for the numerical capabilities of
 886 the sharp and diffuse interface approaches, with the physically observed transition between different
 887 flow regimes during the flow development. Therefore, in Figure 19 are presented the Weber and
 888 Reynolds numbers for the dispersed secondary droplets after impact, which are subject to an
 889 aerodynamic breakup induced by the relative velocity between the injected droplet with calculated
 890 diameter d_z and the expelled surrounding air. As illustrated for successive time instances, the flow
 891 development after impact is restricted by the limit of Ohnesorge numbers less than 0.1, which
 892 indicates that the produced secondary droplets breakup is mainly controlled by the droplet Weber
 893 number (Guildenbecher, Lopez-Rivera and Sojka, 2009). Additionally, only inside the diffuse interface
 894 region are observed Weber numbers with values larger than 0.5, which correspond to the beginning
 895 of the droplets oscillation and deformation (Guildenbecher, Lopez-Rivera and Sojka, 2009), confirming
 896 that the flow topology detection predicts accurately the dispersed flow region. Within the diffuse
 897 interface region and closer to the edges of the radially expanding cloud of secondary droplets are
 898 detected regions with increasing Weber number and values larger than 10, which is set as a limit for
 899 the droplet aerodynamic breakup (Guildenbecher, Lopez-Rivera and Sojka, 2009).



900

901 Figure 19 Droplet fragmentation with impact velocity 150m/s (case 2). Blue iso-surface represents the sharp interface regions
 902 and grey iso-surface the diffuse interface regions calculated with the multiscale two-fluid approach. (on the left) The Weber
 903 number field for the aerodynamic breakup of the produced secondary droplets after impact. Black iso-line corresponds to
 904 Weber number value of 0.5. (on the right) The Reynolds number field for the aerodynamic breakup of the produced
 905 secondary droplets after impact. Red iso-line corresponds to Ohnesorge number value of 0.1.

906 4. Conclusion

907 A compressible Σ -Y two-fluid model with dynamic interface sharpening based on local topological
 908 criteria has been developed and implemented in OpenFOAM[®]. The aim of the present study was to
 909 simulate highly compressible flows with significant slip velocity effects and multiscale complexities
 910 using a uniform solver, which detects dynamically the different coexisting flow regimes and operates
 911 under the most appropriate formulation. The numerically challenging coupling of a two-fluid model
 912 with an interface sharpening method has been examined and validated against a benchmark case of
 913 a shock tube and a rising bubble, obtaining useful results on how eliminating the relative velocity at
 914 the interfacial region to achieve an effective coupling. The overall model functionality has been
 915 thoroughly examined and applied in the highly compressible and multiscale case of a high-speed
 916 droplet impact; new experiments have been performed for a water droplet splashing on a surface at
 917 Weber number $\sim 10^5$ that have not been previously reported in the literature. The obtained results
 918 have shown a good agreement with the conducted experimental study regarding the capturing of the
 919 macroscopic characteristics of droplet fragmentation. Additionally, the proposed model has provided
 920 significant advantages particularly under a dispersed flow regime which dominates the later stages of
 921 droplet splashing in comparison to numerical methods imposing a sharpened interface and thus
 922 excluding all the relevant sub-grid scale phenomena. The developed multiscale two-fluid methodology
 923 contributes with significant additional information regarding the physical phenomenon evolution, like
 924 the relative velocity field, the shock waves development and the interface surface area evolution,
 925 which have contributed to a better understanding and more accurate modelling of complex multiscale
 926 flow fields.

927 Acknowledgements

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 929 Research and Innovation programme under the Marie Skłodowska-Curie Grant Agreement No 675676.

930 Nomenclature

931	α	volume fraction [-]
932	C_α	interface compression coefficient [-]
933	C_D	drag coefficient [-]
934	C_{SGS}	sub-grid scale mechanisms adjustable constant coefficient [-]
935	d	diameter [m]
936	Δt	computational time step [s]
937	e	specific internal energy [kJ/kg]
938	E	interfacial energy source term [W/m ²]
939	F_D	drag force [N]
940	$F_{D\alpha}$	artificial drag force [N]
941	F_s	surface tension force [N]
942	g	acceleration of gravity [m/s ²]
943	k	specific kinetic energy [kJ/kg]
944	κ	interface curvature [1/m]
945	M	interfacial momentum source term [Pa/m]
946	ν	kinematic viscosity [m ² /s]

947	v_{topo}	topological parameter [-]
948	Oh	Ohnesorge number [-]
949	p	pressure [Pa]
950	\mathbf{q}^{eff}	effective heat flux vector [W/m]
951	R_{al}	turbulent liquid flux
952	R_{Σ}	turbulent flux of interface surface area density
953	Re	Reynolds number [-]
954	ρ	density [kg/m ³]
955	σ	surface tension coefficient [kg/s ²]
956	Sc	Schmidt number [-]
957	Σ	liquid gas interface surface area density [1/m]
958	Σ^*	equilibrium liquid gas interface surface area density [1/m]
959	Σ_{min}	minimum liquid gas interface surface area density [1/m]
960	$\boldsymbol{\tau}^{\text{eff}}$	effective stress tensor [Pa]
961	τ_r	artificial drag force relaxation factor [-]
962	τ_{SGS}	sub-grid scale mechanisms time scale [1/s]
963	u	velocity field [m/s]
964	u_c	artificial compression velocity field [m/s]
965	u_r	relative velocity field [m/s]
966	We	Weber number [-]
967	y^+	dimensionless wall distance [-]
968	ψ	compressibility [s/m]

969 **Subscripts**

970	g	gaseous phase
971	l	liquid phase
972	m	liquid and gaseous mixture
973	SGS	sub-grid scale component
974	t	turbulent component

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