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23 the controlling parameter, while the Re number affects the droplet breakup at low We number
24 conditions. The inclusion of droplet heating and evaporation mechanisms has revealed that
25 heating effects have generally a small impact on the phenomenon due to its short duration
26 except for low We number cases. Droplet deformation enhances heat transfer and droplet
27 evaporation. An improved 0-D model is proposed, able to predict the droplet heating and
28 vaporization of highly deformed droplets.

29 **Keywords:** droplet breakup; VOF; heating; evaporation

30

31 **1 Introduction**

32 Droplet breakup and evaporation are important physical processes controlling the efficiency of
33 combustion systems; they are also realised in medical and agricultural applications among
34 others. Due to their importance they have attracted the scientific interest; but generally they
35 have been studied independently. The droplet breakup has been addressed (selectively) in
36 review studies as in [1, 2] and droplet evaporation in the review articles by [3, 4] as also in
37 textbooks like [5, 6] among many other.

38 The aerodynamic droplet breakup induced by an initial relative velocity $U_{rel,0}$ between the
39 droplet and the ambient gas is characterized by different breakup modes depending on the
40 relative strength of the forces acting on the droplet. For a certain configuration, increasing the
41 relative droplet-gas velocity results in different breakup regimes namely a) the bag breakup, b)
42 the transitional or multimode breakup (including the bag-stamen, dual-bag and plume/shear
43 regimes), c) the sheet-thinning breakup termed also sheet-stripping or shear breakup and d) the
44 catastrophic breakup. A qualitative description of these breakup regimes can be found in the
45 aforementioned review studies for droplet breakup as in Guildenbecher et al. [1] among many
46 others. Except for the drop-gas relative velocity, other important parameters affecting the

47 aerodynamic droplet breakup are the material (gas and liquid) properties and the droplet
 48 dimensions. All these can be grouped into dimensionless numbers, namely the Weber number
 49 (We), the Reynolds number (Re), the Ohnesorge number (Oh), the density ratio (ε) and the
 50 viscosity ratio (N), while under certain flow conditions the Mach number and the turbulence
 51 levels may also become important:

$$We = \frac{\rho_g U_{rel,0}^2 D_0}{\sigma} \quad Re = \frac{\rho_g U_{rel,0} D_0}{\mu_g} \quad Oh = \frac{\mu_l}{\sqrt{\rho_l \sigma D_0}} \quad \varepsilon = \frac{\rho_l}{\rho_g} \quad N = \frac{\mu_l}{\mu_g} \quad (1)$$

52 Experiments have shown that the We number is the most influential parameter and thus, most
 53 studies aim to define the critical We number leading to the different breakup regimes. The
 54 critical We is mainly a function of the Oh number and increases for high viscosity liquids
 55 ($Oh > 0.1$); the effect of the rest of the dimensionless numbers is not yet quite clear since the
 56 majority of the experimental studies have examined relatively high Re numbers and density
 57 ratios, above 1000 and 600 respectively; a few exceptions examined $500 < Re < 1000$ and
 58 $80 < \varepsilon < 200$ [7, 8].

59 For the non-dimensionalisation of time, the shear breakup timescale t_{sh} proposed by Nicholls
 60 & Ranger [9] is widely used:

$$t_{sh} = \frac{D_0}{U_{rel,0}} \sqrt{\varepsilon} \quad (2)$$

61 Several experimental studies have investigated the aerodynamic droplet breakup by using the
 62 shock tube and the continuous air jet flow techniques (see details in [1] among others).
 63 Krzeczowski [10] was one of first who presented a detailed breakup map in the We - Oh plane
 64 followed later by the studies of Hsiang & Faeth [11-13] who extended it to higher Oh numbers
 65 up to 560. Subsequent experimental studies aimed to clarify the physical mechanisms behind
 66 the breakup regimes [7, 8, 14] and provided useful information regarding the critical We
 67 numbers leading to different breakup regimes [15, 16], the temporal properties and the size

68 distribution of the child droplets after the parent droplet disintegration [15, 17] and the gas flow
69 structure during droplet breakup [18].

70 Generally, there is a scattering of the experimental data which is probably due to the variety of
71 the experimental techniques used and the experimental uncertainties. Complimentary to the
72 experimental techniques, a large number of numerical works have been performed to enlighten
73 the complicated breakup phenomenon such as those of [19-23]. These studies examined the
74 isothermal droplet breakup in 2D and 3D computational domains and provided insight into the
75 physics behind droplet breakup [19, 20, 22, 23], the effect of parameters other than the We
76 number [19] (Re number, density and viscosity ratio), the droplet drag coefficient [21, 23] and
77 the size distribution of droplets after breakup [23].

78 Regarding the evaporation modelling, several simplified 0-D and 1-D models have been
79 proposed to predict the evaporation of isolated spherical droplets. Starting from the classical
80 “ D^2 -law” of Godsave [24] and Spalding [25], various approaches have been proposed to include
81 the transient droplet heating by prescribing the internal temperature distribution as in [26-31]
82 and the Stefan flow effects as in Abramzon & Sirignano [28] and Yao et al. [32]. The
83 performance of these models was assessed in comparative studies such as those of [33-36] and
84 defined their range of applicability. These models are restricted to spherical droplets and only
85 few exceptions [37-40] have investigated the evaporation of deformed droplets (mainly the
86 oscillatory deformation). Apart from the simplified models which are suitable for the stochastic
87 prediction of the spray performance in Lagrangian models due to their simplicity and reduced
88 computational cost, detailed CFD models [41-44] for single component evaporation and [45-
89 48] for multicomponent droplet evaporation, have been used to give insight on the physical
90 mechanisms occurring during droplet evaporation by solving both the liquid and the gas phase.

91 The coupled problem of droplet breakup and droplet evaporation has not yet been studied
92 thoroughly; only a few CFD studies have examined the heating and evaporation of deformed

93 droplets at low We numbers. Haywood et al [49, 50] were one of the first who examined the
94 evaporation of deformed droplets. They used an adaptive grid fitted to the droplet surface which
95 could predict its deformation but not the breakup. They examined n-heptane droplets in a high
96 temperature gas (1000K) at moderate Re numbers ($10 < Re < 100$) and low We numbers ($We < 10$).
97 They showed that when using a volume-equivalent diameter, the quasi-steady correlations for
98 the Nusselt (Nu) and Sherwood (Sh) numbers can also be used for droplets under steady or
99 unsteady (oscillatory) deformation. On the contrary, the drag coefficient is influenced by the
100 droplet shape and it is a function of Re and We numbers; if the instantaneous dimensionless
101 droplet frontal area is known, then the classical 0-D correlations can be used by multiplying
102 them with this parameter. Mao et al. [51] used a body fitted grid to study the mass transfer of
103 deformed droplets for $We < 8$. They concluded that the Peclet (Pe) number followed by the Re
104 number are the controlling parameters, while the We number has a small impact on the droplet
105 evaporation rate evolution only at very high Pe numbers. Hase & Weigand [52] used a 3D VOF
106 methodology to study the heat transfer enhancement (without evaporation) due to the
107 deformation of hot droplets carried by a colder air stream at high Reynolds numbers
108 ($360 < Re < 853$) and $We < 11$. They found a significant dependency of Nu on We number at the
109 highest Re number case, but to our opinion this conclusion might have been affected by the fact
110 that the heat transfer coefficient was estimated by using the surface area of a sphere. They have
111 also shown that the heat transfer increases not only due to the droplet oscillatory motion but
112 also due to the larger surface area of the deformed droplet; in addition, the transient Nu number
113 at the beginning of the simulation is much higher compared to the steady-state Nu number given
114 by classical correlations. In a follow-up study, the same group [53] included evaporation in
115 their model (as in [44]) and examined the coupled problem of droplet deformation and
116 evaporation. They studied cases including initially spherical or deformed droplets and also
117 isothermal and evaporating cases with the presence of heat transfer from the hot ambient air.
118 The dimensionless numbers examined were in the range of $173 < Re < 347$ and $2.3 < We < 7.8$. They
119 found that the flow field inside the droplets is affecting the droplet heating; the oscillatory

120 droplet movement causes a “sucking” of hotter fluid from the droplet surface towards its centre.
121 They have also identified large temperature differences along the droplet surface which
122 influences the mass transfer and may induce a thermo-capillary flow; however this mechanism
123 was not modelled. Cerqueira et al. [54] studied the interfacial heat and mass transfer in spherical
124 and deformed rising bubbles for $Re < 80$ with the VOF methodology. It was shown that the shape
125 distortion results in decrease of the transfer coefficient and increase of the interfacial area,
126 compensating the effect on the total interfacial flow; the latter becomes dominant in highly
127 distorted particles.

128 The present numerical work aims to fill the gap in literature concerning the coupled problem of
129 droplet breakup in a high temperature environment accounting for the droplet heating and
130 evaporation. The effect of heating and evaporation on droplet breakup is quantified by
131 comparing non-isothermal against isothermal cases at the same flow conditions. The numerical
132 model employs the VOF methodology coupled with the solution of the energy equation, while
133 a local evaporation model is used, which is independent of the droplet shape. The following
134 sections include initially a brief description of the numerical methodology and the cases
135 examined, followed by the results under isothermal and evaporating conditions. The
136 conclusions of the present work are summarized at the end.

137

138 **2 Numerical model and methodology**

139 The numerical model solves the Navier-Stokes equations in a 2D axisymmetric domain and
140 uses the VOF methodology to track the liquid-gas interface. To account for the droplet heating
141 and evaporation, the energy and vapour transport equations are also solved, while the
142 evaporation mass flux is obtained by using a local evaporation model independent of the
143 interface shape, assuming that the computational cells at the liquid-gas interface are saturated.
144 For the non-isothermal cases, the pure species properties are assumed to be a function of

145 temperature according to [55, 56] and the gas mixture properties are taken as mass-averaged
146 based on the vapour concentration assuming incompressible ideal gas.

147 The complete set of the equations solved were in detail presented in Strotos et al. [57] and will
148 not be repeated here. The model has already been validated against a wide range of cases and
149 thus it can be considered to be reliable. These include the motion of a free falling droplet in
150 Malgarinos et al. [58], the aerodynamic breakup of droplets in Strotos et al. [59, 60], the
151 evaporation of single- and multi-component droplet in a high temperature environment in
152 Strotos et al. [57], but also droplet impact onto a solid substrate in Malgarinos et al. [61].

153 The platform provided by the CFD tool ANSYS FLUENT v14.5 [62] was utilized for solving
154 numerically the flow equations; the implicit VOF solver was adopted, which has a robust
155 behavior and allows for higher timesteps when compared to the explicit solver. A number of
156 User Defined Functions (UDFs) were developed and implemented allowing for simulation of
157 the droplet vaporization during their break-up process. These include (apart from the
158 evaporation model and species properties) an automatic local grid refinement technique [61,
159 63], a sharpening algorithm [59] and also the implementation of variable timestep based on a
160 Courant number (C) equal to 0.5 at the interface region; this is a minor change relative to our
161 previous work reported in Strotos et al. [59, 60], in which the Courant number was calculated
162 in the whole computational domain rather than on the interface. The following discretization
163 methods have been utilized: the Compressive discretization scheme for the interface tracking,
164 the Second Order Upwind (SOU) discretization for the momentum and energy equations, the
165 First Order Upwind (FOU) for the species transport equations (a higher order scheme may lead
166 to divergence), the Body Force Weighted (BFW) pressure interpolation scheme, the PISO
167 algorithm for the pressure-velocity coupling and the Bounded Second Order Implicit (BSOI)
168 formulation for the temporal discretization (see details in our previous works as also in [62]).
169 Finally, for the implementation of the surface tension force in the momentum equations, the
170 Continuum Surface Stress (CSS) model by Lafaurie et al. [64] was used in order to include the

171 effect of the thermo-capillary flow due to the variation of the surface tension coefficient along
172 the interface. The numerical settings used for the simulations are summarized in Table 1.

173

174 Table 1: Numerical settings used for the simulations.

Equation	Discretization scheme
VOF	Compressive
Momentum	SOU
Energy	SOU
Species	FOU
pressure interpolation scheme	BFW
Pressure-velocity coupling	PISO
time discretization	BSOI

175

176

177

178 **3 Results and discussion**

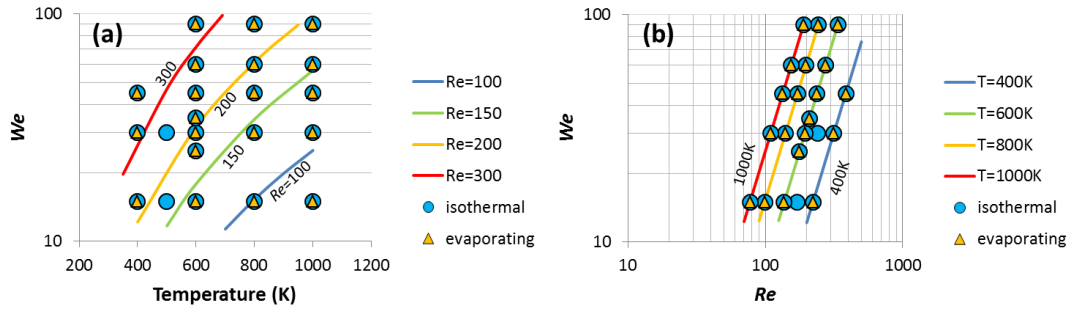
179 **3.1 Cases examined and numerical setup**

180 The cases examined involve a small ($D_0=100\mu\text{m}$) volatile n-heptane droplet subjected to a step
181 change of the gas phase velocity. The droplet has an initial temperature of $T_0=300\text{K}$ which
182 corresponds to $Oh=0.01$ and ensures that the breakup regime is not depending on the Oh

183 number; the Oh number was kept constant for all cases examined. The ambient pressure is
184 atmospheric which ensures the validity of the evaporation model and no high pressure
185 modifications were required. The gas phase velocity is modified so as to achieve We numbers
186 in the range 15 up to 90, while the free stream temperature is varying in the range of 400-
187 1000K; for a given temperature, the gas properties are first calculated and then the gas phase
188 velocity is obtained from the We number definition. Altering the free stream temperature results
189 in density and viscosity ratios in the range of $\varepsilon=770-1926$ and $N=9.1-16.5$, respectively, which
190 according to Aalburg [65] are high enough (well above $\varepsilon>32$) to affect the breakup outcome.
191 Note also that the critical n-heptane temperature is 540K and the present model has been already
192 validated from the authors against supercritical temperatures in Strotos et al. [57].

193 The aforementioned combinations of We number and free stream temperatures, led to high free-
194 stream velocities in the range of 57-223m/s, but the compressibility effects are negligible since
195 the maximum Mach number is 0.35 (observed for $We=90$). In all cases the Re number is below
196 400 which ensures that the flow remains laminar and the axisymmetric solution is applicable
197 [5, 66]. Nevertheless, in the parametric study conducted in Strotos et al. [60] with the 2D
198 axisymmetric model, the Re numbers examined were much higher without affecting the
199 qualitative model performance.

200 A complete list of the cases examined is shown in Fig. 1 in the $We-T_\infty$ plane and the $We-Re$
201 plane. For the isothermal cases, the energy equation and the evaporation source terms were not
202 accounted for and the species properties were kept constant at their reference temperature
203 values, i.e. at $T_0=300K$ for the liquid droplet and at T_∞ for the surrounding air; namely,
204 isothermal runs correspond to a parametric study for the effect of We and Re numbers.



205

206 Fig. 1: Cases examined in (a) the $We-T_\infty$ plane and (b) the $We-Re$ plane.

207

208 Regarding the computational domain and the boundary conditions, these are the same as in
 209 Strotos et al. [59, 60]. Briefly, the droplet is initially motionless and it is subjected to a step
 210 change of the gas phase velocity. The grid is moving with the average droplet velocity and
 211 upstream the droplet a fixed absolute velocity and temperature is applied (Dirichlet boundary
 212 condition), while downstream a zero first gradient boundary for all variables is used. The
 213 unstructured grid has a density of 192 cells per radius (cpR) at the interface region and it is fine
 214 enough to resolve the boundary layers. More specifically, in Feng & Michaelides [67] it is
 215 stated that the hydrodynamic boundary layer thickness is proportional to $Re^{-1/2}R$; for $Re=400$ it
 216 has a thickness of $0.05R$. For the highest Re number examined here, there are 9-10
 217 computational cells inside the boundary layer region, which can be considered a realistic grid
 218 resolution for VOF simulations suitable for the present runs.

219

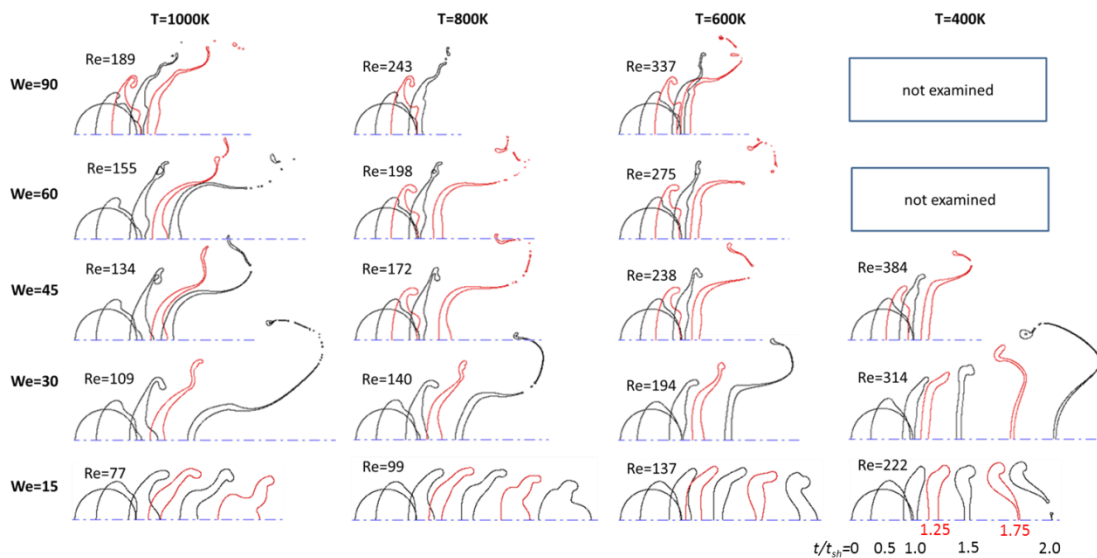
220 3.2 Isothermal cases

221 3.2.1 General breakup behaviour

222 The results obtained for the droplet shapes assuming isothermal flow conditions and constant
 223 properties are shown in Fig. 2. The droplet shapes drawn in black correspond to time intervals

224 of $0.5t_{sh}$ (i.e. 0.0, 0.5, 1.0, 1.5, $2.0t_{sh}$) and the droplets drawn in red correspond to intermediate
 225 instances i.e. 0.75, 1.25, 1.75, $2.25t_{sh}$ (the time instant of $0.25t_{sh}$ has been omitted); the last
 226 droplet shape corresponds to the instant of breakup. For a direct correspondence to Fig. 1b, the
 227 We number increases from bottom to top and the gas phase temperature from right to left. With
 228 this arrangement, the Re number increases from bottom to top and from left to right. These runs
 229 verify that the We number is the controlling parameter. Increasing the We number results in
 230 different breakup regimes, namely bag breakup for $We=15$, multimode breakup for $We=30-60$
 231 and sheet thinning breakup for $We=90$. Nevertheless, the transition between the multimode and
 232 the sheet-thinning breakup is not quite clear verifying that breakup is a continuous process [1];
 233 this is also affected by the low Re numbers examined. We have assumed that $We=90$
 234 corresponds to sheet-thinning breakup due to the fact that the droplet breaks up earlier, before
 235 it is subjected to a high stretching. A false three-dimensional representation of the cases
 236 corresponding to $T_\infty=400K$ is shown in Fig. 3.

237

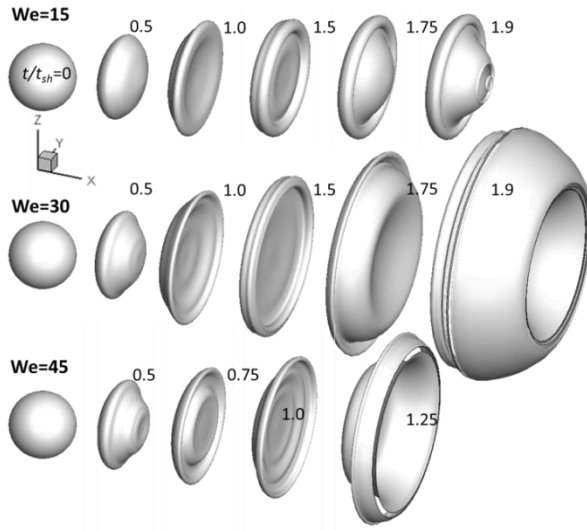


238

239 Fig. 2: Droplet shapes for the isothermal runs. The Re number increases from bottom to top and
 240 from left to right. The droplet shapes drawn black (see the online version) correspond to time

241 intervals of $0.5t_{sh}$ and the droplet shapes drawn red correspond to representative intermediate
 242 instances of $0.25t_{sh}$. The last droplet shape corresponds to the instant of breakup.

243



244

245 Fig. 3: Three-dimensional representation of the droplet shape evolution at three different We
 246 numbers examined for the isothermal cases corresponding to $T_{\infty}=400K$.

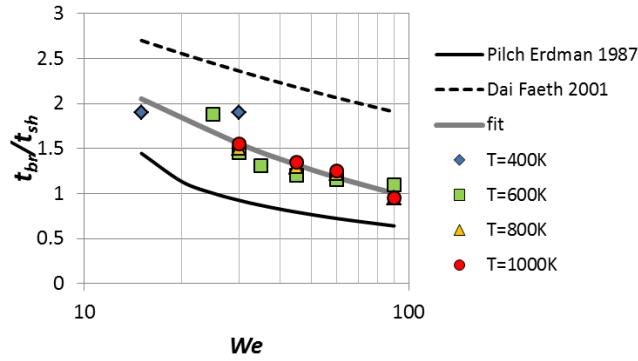
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248 As already stated in section 3.1, the density and the viscosity ratios examined are high enough
 249 so that do not affect the results; thus, the Re number is the remaining parameter affecting the
 250 outcome for the isothermal runs. Earlier numerical studies have shown that there is a
 251 dependency on Re number for $Re < 100$ [65]. The present simulations for $77 < Re < 385$ have
 252 shown that decreasing the Re number does not alter the breakup outcome, but results in a
 253 slightly higher deformation of the liquid structure for intermediate We numbers in the range 30-
 254 60. On the other hand, the effect of Re number at the lowest We number case of $We=15$ should
 255 be emphasized. It is clear that there is a critical Re number between 137 and 170 (the latter was
 256 obtained for $T_{\infty}=500K$), below which no breakup is observed; it can be assumed that for $We=15$
 257 and $Oh=0.01$ the critical Re number is 155 (an average of the aforementioned numbers). This

258 fact was also observed in the numerical work of Han & Tryggvason [19] and it is also stated in
259 the review article of Guildenbecher et al. [1] that there is a dependency on Re number in the
260 bag breakup regime. In any case, one should have in mind that the 2D axisymmetric simulations
261 performed in this study ignore three-dimensional effects which probably alter the phenomenon
262 at the last stages near the breakup.

263 The predicted dimensionless breakup time (the so-called “initiation time”) for the isothermal
264 cases is shown in Fig. 4, along with the corresponding experimental correlations given by Pilch
265 & Erdman [68] and Dai & Faeth [15]. The temperatures appearing in the legend of Fig. 4
266 correspond to the hypothetical free stream temperature at which the gas phase properties were
267 calculated; so for the same We number, a different temperature indicates a different Re number.
268 The predicted breakup time lies between the experimental correlations and correctly predicts
269 the faster breakup with increasing We number, while there is only a weak dependency on Re at
270 low We numbers. However, the experimental correlations are subjected to several uncertainties
271 regarding the estimation of the initiation time as Khosla & Smith [20] stated; moreover, our
272 estimation of the breakup time is subjected to errors in the order $0.05t_{sh}$ (2.5-5%) since this is
273 manually obtained by examining post-processed images. Despite the aforementioned
274 uncertainties, the general trend is correctly predicted and a best fit curve representing our results
275 is $t_{br}/t_{sh}=6.06We^{-0.4}$. Generally the duration of the phenomenon is short and in dimensional units
276 it lasts 20-100 μ s for the examined cases.

277



278

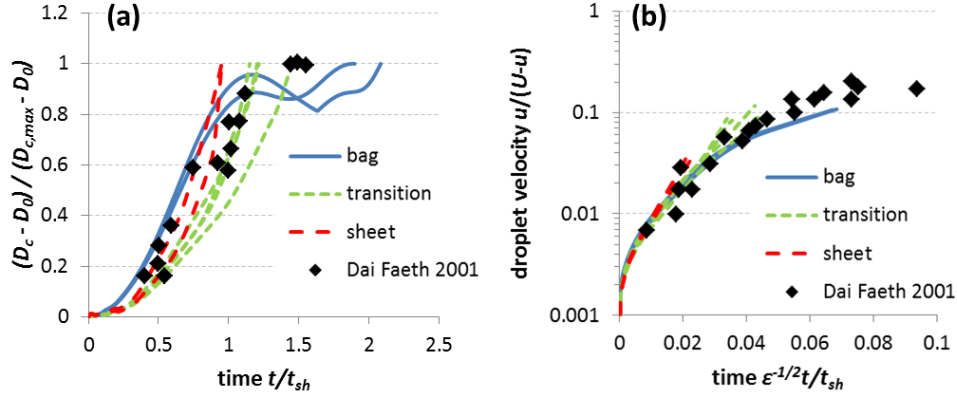
279 Fig. 4: Predicted dimensionless breakup time for the isothermal cases.

280

281 3.2.2 Measured quantities during breakup

282 The temporal evolution of the droplet's cross-stream diameter (D_c) and velocity are given in
 283 Fig. 5 (a) and (b) respectively for selected cases corresponding to bag, transitional and sheet-
 284 thinning breakup. The axes of the graphs have been non-dimensionalized as in Dai & Faeth
 285 [15], thus allowing for a direct comparison with their experimental data and showing a good
 286 qualitative agreement; here u represents the instantaneous droplet velocity and U the free stream
 287 gas phase velocity. As seen, the droplet's cross-stream diameter after a short non-deforming
 288 period of approximately $0.3t_{sh}$ starts to increase almost linearly with time, in agreement with
 289 the experimental findings of Cao et al. [16]. Nevertheless, the present results show a slightly
 290 different behaviour at the later stages of the bag breakup in which the cross-stream diameter
 291 stabilizes near its maximum. This is attributed to the low Re number case, since our simulations
 292 for high Re numbers in [60] shows a continuously increasing deformation. Regarding the
 293 droplet velocity depicted in Fig. 5b, this increases continuously with time but with a
 294 progressively decreasing rate and agrees with the experimental data of Dai & Faeth [15].

295



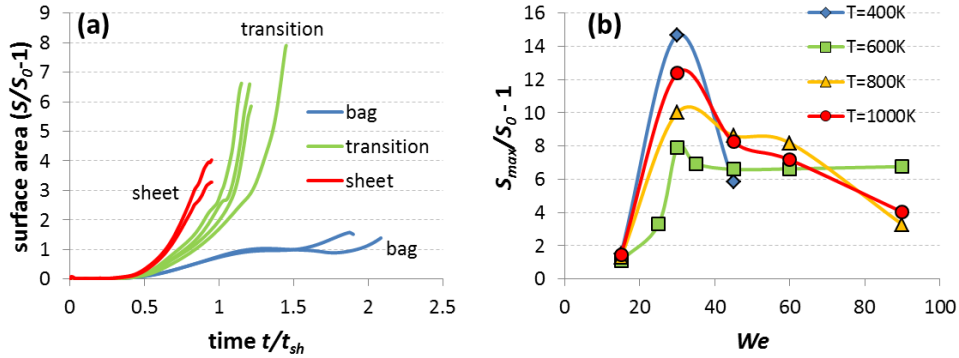
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297 Fig. 5: Temporal evolution of (a) droplet's cross-stream diameter and (b) droplet's velocity for
 298 selected isothermal cases.

299

300 The droplet's surface area (S) is of interest due to its importance in combustion systems;
 301 moreover, it is a quantity which is difficult to measure experimentally. This parameter is shown
 302 in Fig. 6a for selected cases corresponding to the breakup regimes examined. The surface area
 303 is non-dimensionalized with that of a sphere (S_0) having the same volume. As seen in Fig. 6a,
 304 the droplet surface area after the initial non-deforming period starts to increase with a fast rate,
 305 exhibiting dimensionless deformation rates of the order 1.3-8, which increases with increasing
 306 We number; this behaviour is in accordance with the findings of Han & Tryggvason [19]. For
 307 the bag breakup cases ($We=15$), the droplet surface area increases with an almost linear way
 308 (deformation rate ~ 1.3) and at the time instant of breakup it is approximately equal to $2.5S_0$.
 309 For the transitional breakup cases ($We=30-60$), the droplet surface area exhibits a different
 310 behaviour characterised by a higher rate of deformation. After the initial non-deforming period
 311 the droplet surface area increases exponentially and exhibits a high stretching, exceeding values
 312 of $7S_0$. Finally, the sheet-thinning breakup cases exhibit even higher rate of deformation, but
 313 the droplet breaks up earlier and thus the final droplet deformation is lower than that of the
 314 transitional case at the instant of breakup.

315



316

317 Fig. 6: (a) Temporal evolution of the dimensionless droplet surface area for selected isothermal
 318 cases and (b) maximum surface area as a function of We number.

319

320 In the absence of a conservation law for the surface area evolution, the temporal evolution of
 321 droplet surface area can be approximated with the fitting curve of Equation 3 and the
 322 coefficients c_1 and c_2 imply that the rate of deformation increases with increasing We and
 323 decreasing Re number; Equation 3 is valid for $t < t_{sh}$ and the entire range of the isothermal
 324 conditions examined, i.e. $15 < We < 90$, $77 < Re < 385$. It has to be noted that the selection of the
 325 \sinh function in Equation 3 was found to be the most suitable choice among many options
 326 examined including the polynomial, power and exponential; since $\sinh(0)=0$ (which
 327 corresponds to an initially spherical droplet), the initial non-deforming period is reasonably
 328 well predicted and increases with a progressively faster rate.

$$S/S_0 - 1 = c_1 \sinh\left(c_2 \cdot \frac{t}{t_{sh}}\right), \quad t < t_{sh} \quad (3a)$$

$$c_1 = 0.0082We^{0.537} \quad (3b)$$

$$c_2 = 5.47We^{0.136}Re^{-0.138} \quad (3c)$$

329 This curve was obtained by fitting the surface area up to $t=t_{sh}$ since after this time a more
330 complicated function is needed to capture the temporal evolution of the surface area, which
331 may change slope due to the appearance of interfacial instabilities. The fitting curve can be
332 extended up to $t=t_{br}$ (except of the bag breakup cases) to give a rough estimation of the surface
333 area at the instant of breakup. However, our predictions of the surface area at the instant of
334 breakup (see Fig. 6b) have shown that this magnitude is not following a smooth variation when
335 the We and Re numbers are changing, while a local peak at $We=30$ is observed. This is mainly
336 attributed to the error of the estimation of the breakup instant, but also on interfacial instabilities
337 which suddenly alter the rate of deformation. Concluding, Equation 3 should be used with
338 caution for $t_{sh}<t<t_{br}$ and limit the maximum value not to exceed $10-14S_0$, since unphysical
339 values may obtained.

340 The drag coefficient of the deformed droplets is of major interest due to its importance in
341 breakup models. There are various approaches to estimate the drag coefficient. Here we have
342 adopted the correlations given in Pilch & Erdman [68]:

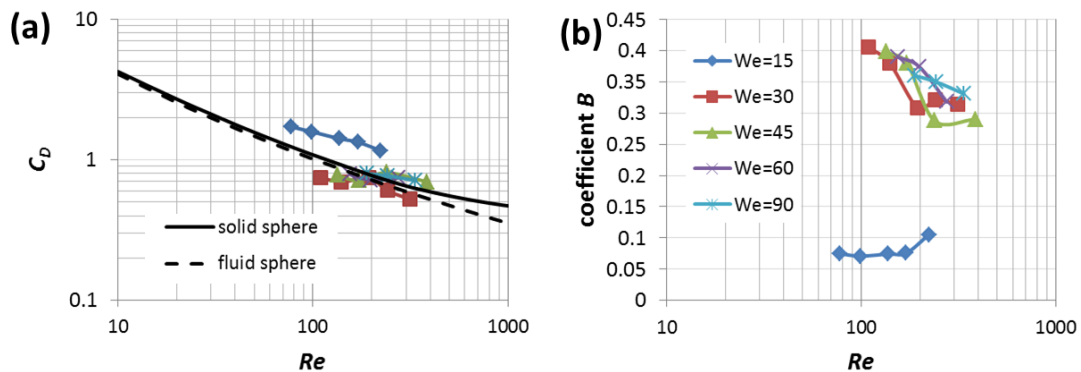
$$\frac{X}{D} = \frac{3}{8}C_D \left(\frac{t}{t_{sh}}\right)^2 + B \left(\frac{t}{t_{sh}}\right)^3 \quad (4)$$

$$\frac{u}{U} \sqrt{\varepsilon} = \frac{3}{4}C_D \left(\frac{t}{t_{sh}}\right) + 3B \left(\frac{t}{t_{sh}}\right)^2 \quad (5)$$

$$\frac{du}{dt} \frac{D \cdot \varepsilon}{U^2} = \frac{3}{4}C_D + 6B \left(\frac{t}{t_{sh}}\right) \quad (6)$$

343 These equations (4-6) are valid for gas-droplet systems (i.e. high density ratios ε), while the
344 coefficient B accounts for the changing of the droplet frontal area and the unsteadiness of the
345 drag coefficient (i.e. $B=0$ would denote a sphere at steady state). Pilch & Erdman [68] assumed
346 $C_D=0.5$ which corresponds to the drag coefficient of a solid sphere for incompressible flow and
347 high Re numbers ($Re>1000$), and fitting the droplet displacement data with Equation 4, they
348 obtained a value of B equal to 0.0758. Here a similar approach is adopted, but without a-priori

349 assuming a value for the drag coefficient. The results obtained for C_D and B are shown in Fig.
 350 7 versus the Re number. The drag coefficient shown in Fig. 7a decreases with the Re number
 351 and it is close to the drag coefficient of a solid sphere [5] and to that of a fluid sphere [67] at an
 352 average viscosity ratio of the cases examined. It has to be noted that the case with $We=15$
 353 exhibits a higher C_D which is due to the hollow spherical shape of the bag breakup. Regarding
 354 the correction coefficient B shown in Fig. 7b, there is a different behaviour depending on the
 355 breakup type. Bag breakup is characterized by low B values (~ 0.07) with a slightly increasing
 356 trend with Re number, while the other breakup regimes are characterized by higher B values
 357 (0.3-0.4) with a decreasing trend with Re number. A better understanding of the trends for the
 358 aforementioned coefficients requires the examination of a wider range of We and Re numbers.
 359



360
 361 Fig. 7: (a) drag coefficient C_D and (b) coefficient B obtained from curve fitting of the droplet
 362 displacement data for the isothermal cases.

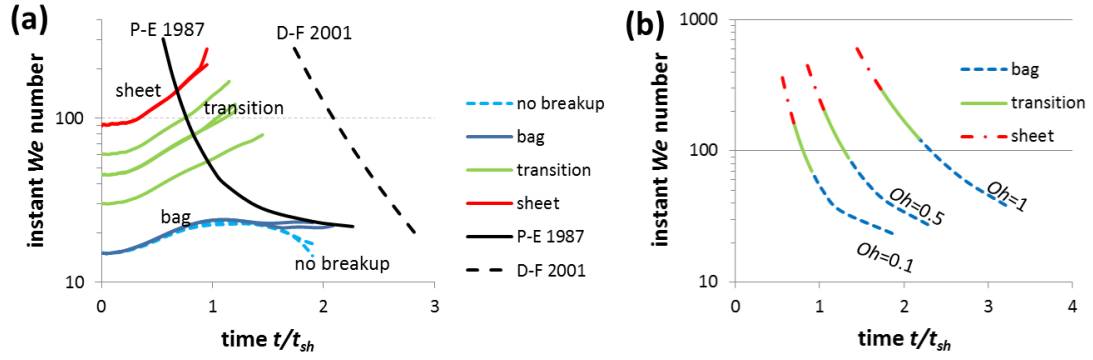
363
 364 It is also interesting to examine the transient ratio of the instantaneous deforming versus the
 365 restorative forces acting on the droplet. Ignoring the viscous forces (since $Oh < 0.1$) this ratio
 366 represents an instantaneous Weber number We_t (aerodynamic vs surface tension forces) defined
 367 with the instantaneous droplet-gas relative velocity $u_{rel,t}$ and the cross-stream diameter $D_{c,t}$ (see

368 Equation 7); the instantaneous droplet-gas relative velocity is obtained by subtracting the
 369 instantaneous volume averaged droplet velocity from the free-stream gas phase velocity.

$$We_t = \frac{\rho_g u_{rel,t}^2 D_{c,t}}{\sigma} = We_0 \left(\frac{D_{c,t}}{D_0} \right) \left(\frac{u_{rel,t}}{U} \right)^2 \quad (7)$$

370 The predicted transient We number based on Equation 7 is plotted in Fig. 8a for selected cases.
 371 It is clear that in the cases which lead to breakup, the deformation forces become progressively
 372 stronger compared to the restorative forces since We_t increases, while in the non-breakup cases,
 373 after reaching a maximum, the deformation forces progressively decrease. Two curves are also
 374 shown in Fig. 8a. These arise from Equation 7 evaluated at the instant of breakup by using
 375 either the breakup time of Dai & Faeth [15] (abbreviated as D-F 2001), or the correlation of
 376 Pilch & Erdman [68] for $Oh=0.01$ (abbreviated as P-E 1987). In both curves the cross-stream
 377 diameter and the relative droplet-gas velocity were obtained from the data of [15]; as seen, the
 378 predicted breakup falls between these two curves. When the two lines cross, breakup occurs.
 379 So, this plot represents a critical instantaneous condition for breakup. The critical instantaneous
 380 conditions for various breakup regimes as a function of the Oh number are shown in Fig. 8b.
 381 This is a qualitative graph obtained by using the breakup time of Pilch & Erdman [68] which
 382 accounts for the effect of Oh number, typical critical We numbers leading to different breakup
 383 regimes (12-35 for bag breakup, 35-80 for transitional and 80 for sheet-thinning), as also the
 384 dependency of the critical We number versus the Oh number; $We_{cr} = We_{cr, Oh \rightarrow 0} (1 + 1.077 Oh^{1.6})$,
 385 $Oh < 10$ from [68]. This graph reveals that increasing the Oh number (i.e. the viscous forces)
 386 requires more time and higher instantaneous aerodynamic forces for breakup to occur;
 387 nevertheless, this cannot be verified in the present work since for all cases examined the Oh
 388 was kept constant to 0.01.

389



390

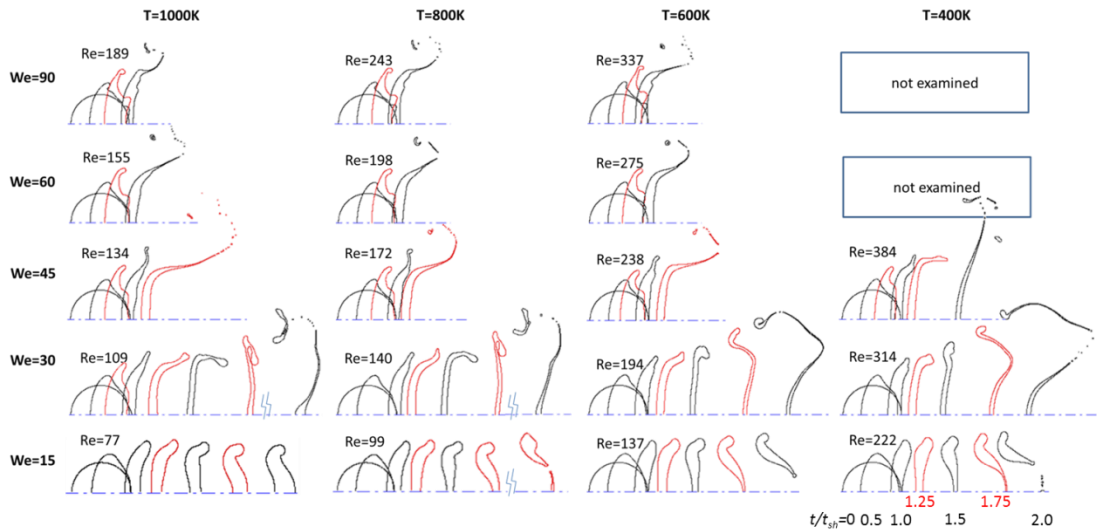
391 Fig. 8: (a) Predicted instant We number for selected isothermal cases and (b) instantaneous
 392 critical breakup conditions for various Oh numbers.

393

394 3.3 Evaporating cases

395 3.3.1 Hydrodynamic behaviour of the droplet

396 Focusing now on the cases including droplet heating and evaporation with variable properties,
 397 the results obtained for the droplet shapes are shown in Fig. 9 using the same pattern as in Fig.
 398 2. Similar to the isothermal cases, the We number is the controlling parameter leading to bag
 399 breakup for low We numbers and multimode breakup for intermediate We numbers ($We=30$ -
 400 60); moreover, we have assumed that $We=90$ corresponds to the sheet thinning breakup due to
 401 the earlier droplet breakup. Compared to the isothermal cases, the droplet heating and
 402 evaporation has a minor effect on the droplet breakup for $We>30$, since quite similar droplet
 403 shapes were obtained. On the other hand, there is a significant influence for the low We number
 404 of 15 case in which droplet breakup is observed for a lower Re number in-between 77 and 99;
 405 it has been assumed that the critical Re number is 88 and while in the isothermal cases the
 406 critical Re was found to be 155. The effect of heating on droplet breakup is that the surface
 407 tension coefficient decreases with a subsequent reduction of the restorative forces; these points
 408 will be further discussed in the following sections of the paper.

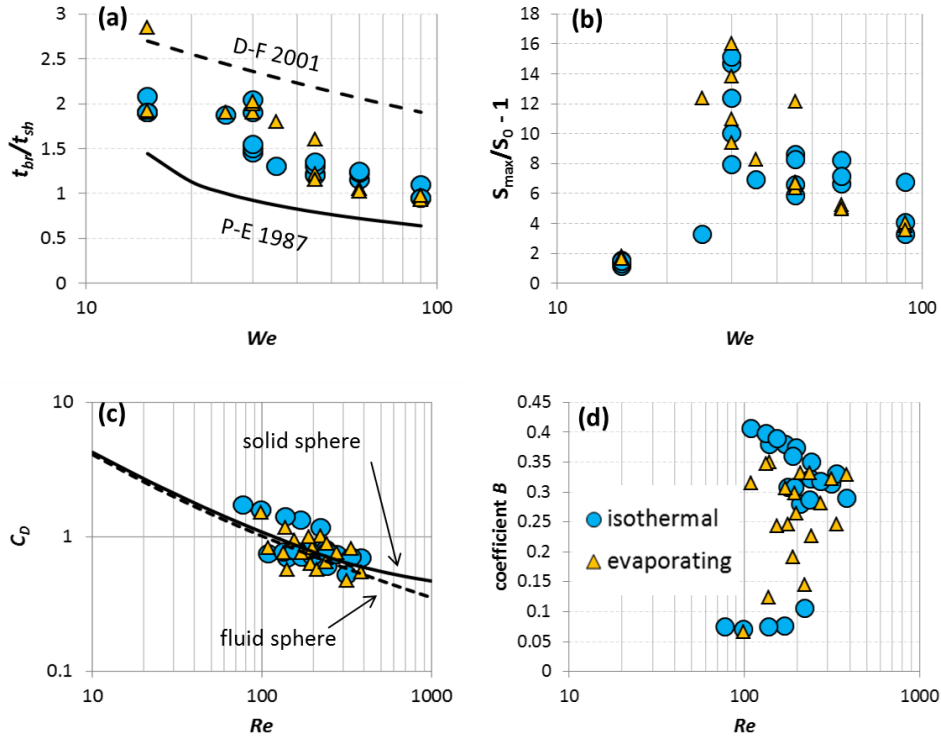


410

411 Fig. 9: Droplet shapes for the evaporating cases. The Re number increases from bottom to top
 412 and from left to right. The droplet shapes drawn black (see the online version) correspond to
 413 time intervals of $0.5t_{sh}$ and the red droplet shapes correspond to representative intermediate
 414 instances of $0.25t_{sh}$. The last droplet shape corresponds to the instant of breakup.

415

416 Regarding the hydrodynamic characteristics of droplet breakup, it seems that these remain
 417 rather unaffected by the droplet heating. The instant of breakup is quite similar in the isothermal
 418 and the evaporating cases with an exception for the case $(We, Re, T)=(15, 99, 800)$ which
 419 requires more time for breakup since it is very close to the “estimated” critical Re number of
 420 88 for bag breakup to occur. The maximum surface area and the drag coefficient are within the
 421 same range of values as in the isothermal cases, but the coefficient B shows a scatter in the
 422 evaporating cases; nevertheless it has the same range of values as in the isothermal cases. A
 423 comparison of the predictions between the isothermal and the evaporating simulations for the
 424 aforementioned quantities is shown in Fig. 10.



425

426 Fig. 10: Comparison of the predictions of the isothermal and the evaporating simulations for
 427 the (a) breakup instant, (b) maximum surface area, (c) drag coefficient and (d) coefficient B .

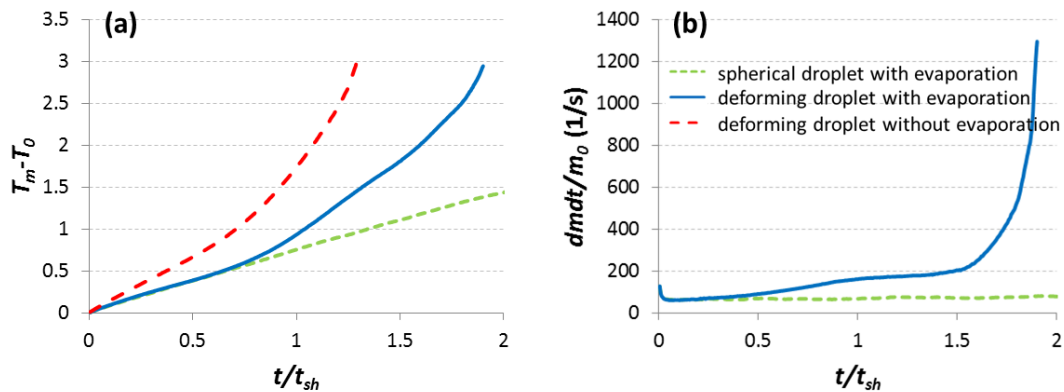
428

429 3.3.2 Thermal behaviour of the droplet

430 Turning now to the thermal characteristics of the cases examined, the temporal evolution of the
 431 volume averaged droplet temperature T_m and evaporation rate dm/dt are presented in Fig. 11a,b,
 432 respectively, for the representative case with $We=30$ and $T_\infty=600K$. In order to assess the effect
 433 of evaporation and the effect of the surface area increase, two more cases are presented in Fig.
 434 11, apart from those mentioned in section 3.1. In the first one, the evaporation source terms
 435 have been omitted (label “deforming droplet without evaporation”) while in the second one, the
 436 surface tension coefficient was artificially increased in order to achieve a nearly spherical
 437 droplet subjected to small shape oscillations (label “spherical droplet with evaporation”).
 438 Comparing the two evaporating cases (deformed and spherical), one can clearly see the effect

439 of droplet deformation which increases the total heat transfer to the droplet due to the surface
 440 area increase. Comparing the deforming cases with and without evaporation, one can clearly
 441 see that evaporation decreases the heat transfer due to the thickening of the boundary layers
 442 (Stefan flow) as also due to the fact that a portion of the heat transferred to the droplet is spent
 443 for phase change. The evaporation rate in Fig. 11b shows that the droplet deformation results
 444 in a more intense increase of the mass transfer from the droplet compared to the spherical
 445 droplet case; nevertheless, due to the short duration of the breakup phenomenon, the total
 446 evaporated mass is in the range 0.3-2.0% of the initial droplet mass for all cases examined and
 447 similarly the volume averaged droplet heat-up is in the range 0.4-7K. Due to the thermal
 448 expansion effect, the droplet volume changes less than the droplet mass and it does not exceed
 449 1% of the initial volume.

450



451

452 Fig. 11: Temporal evolution of (a) volume averaged droplet temperature and (b) evaporation
 453 rate for the case of $(We, T_\infty) = (30, 600)$.

454

455 It is also of interest to estimate the Nusselt (Nu) and Sherwood (Sh) numbers for the heat and
 456 mass transfer respectively and then use them in simplified 0-D models aiming to predict droplet
 457 heating. The Nu and Sh numbers represent the dimensionless temperature and concentration

458 gradients respectively at the droplet interface; earlier studies using body-fitted grids [41, 42]
459 estimated them directly by calculating the gradients at the interface. Nevertheless, this is not
460 straightforward within the framework of the VOF simulations, because of the continuous
461 variation of the field magnitudes at the interface region. As a result, the discontinuities of
462 temperature and concentration gradients at the interface region cannot be captured even with a
463 very fine mesh (see also details in [54]). In order to estimate them, a different approach is
464 adopted which is based on 0-D relationships outlined in equations 8-13. These form an
465 enhanced 0-D model which can also estimate the surface temperature through an additional
466 equation relating the droplet surface temperature with its volume averaged one; this was
467 inspired by the work of Renksizbulut et al. [29]:

$$\rho_l V \frac{d(c_{p,l} T_m)}{dt} = S \left(\frac{Nu \cdot k_{g,\infty}}{D_0} (T_\infty - T_s) - \dot{m}'' L \right) \quad (8)$$

$$\dot{m} = S \frac{Sh \cdot \rho_{g,\infty} D_{AB,\infty}}{D_0} \ln(1 + B_M) \quad (9)$$

$$Nu_l \cdot k_{l,0} \frac{T_s - T_m}{D_0} = Nu \cdot k_{g,\infty} \frac{T_\infty - T_s}{D_0} - \dot{m}'' L \quad (10)$$

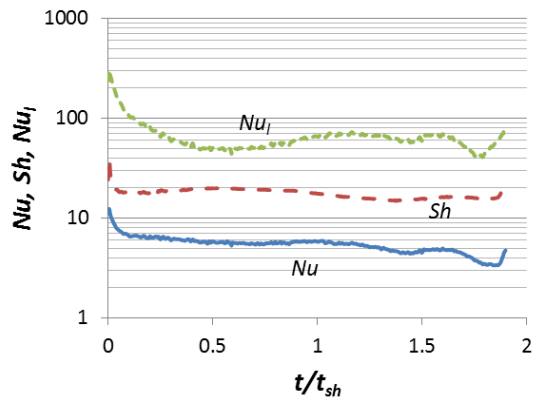
$$\overline{Nu} = \frac{2 + 1.18 Re_\infty^{0.346} Pr_{g,\infty}^{1/3}}{(1 + B_{T,\infty})^{0.7}} \quad (11)$$

$$\overline{Sh} = \left(2 + 0.062 Re_\infty^{0.915} Sc_{g,\infty}^{1/3} \right) (1 + B_{T,\infty})^{0.6} \quad (12)$$

$$\overline{Nu}_l = 53.63 + Re_l / 59.62 \quad (13)$$

468 Equation 8 is the overall droplet energy balance; Equation 9 is a commonly used relationship
469 for the evaporation rate and Equation 10 is the heat flux continuity at the droplet's surface, in
470 which Nu_l represents the dimensionless temperature gradient from the liquid side; this equation
471 connects the average droplet temperature T_m with the surface temperature T_s . Using the CFD
472 data for the mean droplet temperature T_m , the spatial average surface temperature T_s and the

473 evaporation rate dm/dt , from equations 8-10, one can solve for Nu , Sh and Nu_l numbers and
 474 find their variation with time; a similar concept was used by Hase & Weigand [52] in order to
 475 obtain the Nu number but without evaporation. This is shown in Fig. 12 for the case
 476 $(We, T_\infty)=(30, 600)$ which can be regarded as representative, since the qualitative characteristics
 477 observed apply to all cases examined. The Nu and Sh numbers after a short initial transitional
 478 period related to the development of the flow fields around and inside the droplet, remain almost
 479 constant with time. The Nu_l number has a more unsteady character. It exhibits a larger variation
 480 of almost one order of magnitude and has a longer transitional period when compared to the
 481 corresponding Nu and Sh . The short initial transient behavior of the transfer numbers is in
 482 agreement with the one calculated in [41, 42, 52].



483

484 Fig. 12: Temporal variation of Nu , Sh and Nu_l for the case of $(We, T)=(30,600)$.

485

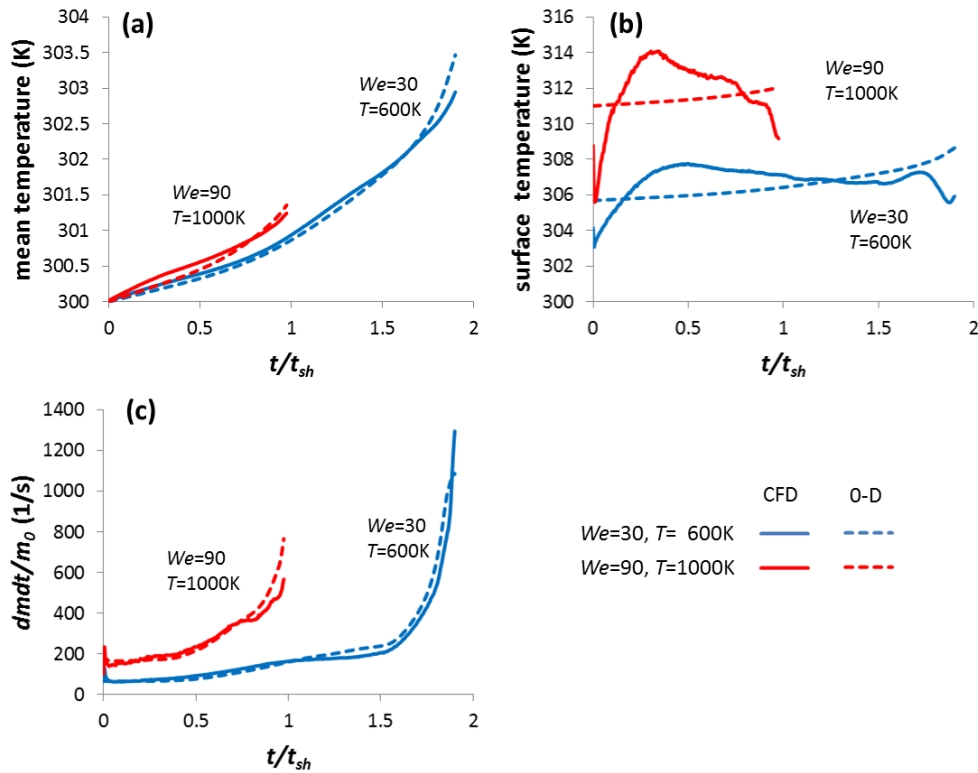
486 Earlier CFD works on spherical droplet evaporation [41, 42] gave expressions of the Nu and Sh
 487 numbers as a function of the instantaneous Re , Pr and Sc numbers. Nevertheless, this is not
 488 applicable in the present work, since the duration of the phenomenon is short without any
 489 appreciable changes of the droplet velocity and temperature. Thus, it was considered more
 490 efficient to use time-averaged expressions based on the free-stream dimensionless numbers.
 491 The time-averaged \overline{Nu} , \overline{Sh} and $\overline{Nu_l}$ numbers are given in eq 11-13 and they can be used in

492 equations 8-10 instead of the corresponding instantaneous to predict the temporal evolution of
493 the droplet temperature and evaporation rate with sufficient accuracy; this is shown in Fig. 13
494 for two cases combining different We numbers and gas phase temperatures. As seen, the model
495 predictions for the average droplet temperature and the evaporation rate are satisfactory, while
496 for the surface temperature there are discrepancies due to the fact that Nu_l has a more transient
497 character, which is ignored when a time-averaged expression is used. Nevertheless, this
498 enhanced model is able to provide the additional information of surface temperature and
499 correctly predicts the trends of the evaporation rate and the average droplet temperature with
500 less than 0.5K error. For the surface temperature T_s , the initial condition used was to set it equal
501 to the contact temperature between semi-infinite solids [69] and this concept was also used in
502 [70-72] for droplet impact on hot substrates. The initial condition for the surface temperature is
503 shown in Equation 14 and agrees well with the CFD predictions at the first time-step.

$$T_{s,0} = \frac{\gamma_l T_0 + \gamma_g T_\infty}{\gamma_l + \gamma_g} \quad (14)$$

504

505



506

507 Fig. 13: Predictions of the 0-D model for (a) the volume averaged droplet temperature, (b) the
 508 surface temperature and (c) the evaporation rate. Solid lines are the CFD data and dashed lines
 509 are the 0-D model predictions.

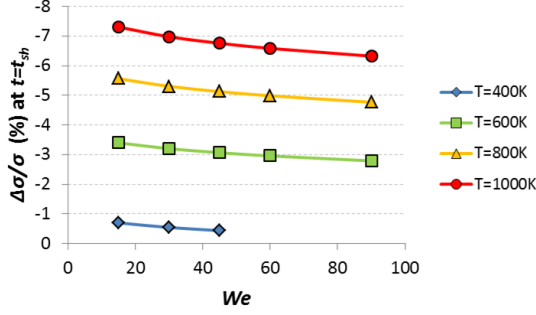
510

511 Some further comments should be made for the set of equations 8-13. As the proposed
 512 correlations represent time-average parameters, they are using the free-stream properties and
 513 not film conditions, they are based on initial dimensionless numbers and do not account for
 514 their temporal variation since the duration of the phenomenon is short. Under these
 515 assumptions, the proposed correlations cannot be directly compared against others referring to
 516 spherical droplets. Another limitation of the proposed 0D model, is that it requires the
 517 knowledge of the temporal variation (history) of the droplet surface area. This can be done by
 518 using Equation 3 for the temporal variation of the surface area, but more work is needed to
 519 obtain the corresponding coefficients, since for the case of droplet evaporation they also depend

520 on the droplet heat-up. For the case in which the temporal evolution of the surface area is not
521 known, one can obtain qualitative but less accurate results, by using the surface area of a sphere
522 in Equations 8 and 9 and multiplying the \overline{Nu} and \overline{Sh} numbers with the correction factors
523 $\{1.28 + 0.7\exp(-0.07|We - 30|)\}$ and $\{1.6 + 1.3\exp(-0.07|We - 30|)\}$ respectively;
524 these are valid for supercritical ambient temperatures ($T_\infty > 600\text{K}$). A final comment should be
525 made for the equation describing the averaged Sh number (Equation 12), which was found to
526 be related with B_T and not the Spalding number B_M , since the initial droplet temperature and
527 the liquid species were fixed in the present work. Additionally, the Nu_l number in Equation 13
528 should be normally related to the liquid properties (e.g. the Pr_l number), but this is not
529 applicable in the present study since only one liquid species was examined. The Re_l appearing
530 in Equation 13 was taken from [73] and it is calculated as $Re_l = Re_\infty \varepsilon^{2/3} N^{-4/3}$.

531 Using the proposed 0-D model (equations 8-13) and the surface area variation according to
532 Equation 3 (extended up to the breakup instant and limited up to $S_{max}=10S_0$), one can estimate
533 initially the surface temperature at $t=t_{sh}$ and then the percentage change of the surface tension
534 coefficient σ , which has an important effect of the droplet heating; this is shown in Fig. 14, in
535 which the vertical axis values are presented in reversed order, and it is in agreement with the
536 corresponding CFD data at the same time instant. As seen, the relative change of surface tension
537 coefficient becomes important either for low We numbers or for high ambient temperatures, as
538 expected; it will not alter the breakup characteristics at high We cases. On the other hand, at the
539 low We number of 15 and $T_\infty=600\text{K}$, the reduction of the surface tension coefficient by 3.5% is
540 enough to lead to breakup; note that in this specific case the droplet was not breaking up under
541 isothermal conditions. Finally, for a less volatile fuel than the examined n-heptane, the
542 reduction of surface tension coefficient is expected to be higher due to higher heating and this
543 is a subject of future work.

544



545

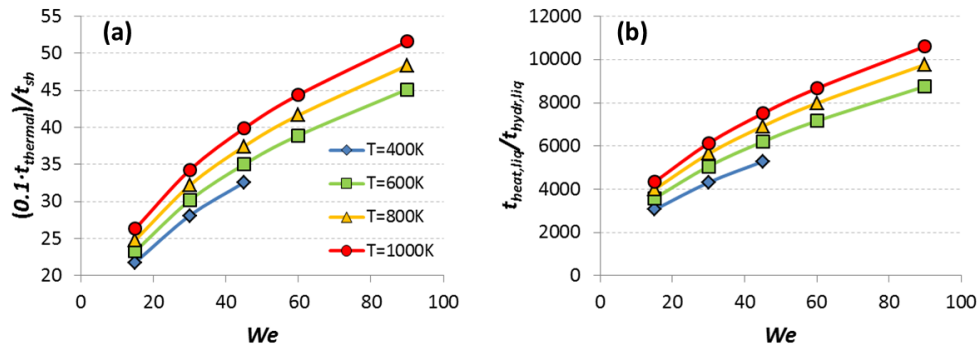
546 Fig. 14: 0-D model predictions for the percentage change of surface tension coefficient at $t=t_{sh}$
 547 as a function of We number and gas phase temperature.

548

549 Complimentary to the discussion about the reduction of the surface tension coefficient, the
 550 minor impact of droplet heating on the breakup of a volatile fuel droplet (except of the low We
 551 number cases) can be explained by comparing the associated timescales, either in a macroscopic
 552 or in a microscopic level. In a macroscopic level, the associated timescales are the shear breakup
 553 timescale t_{sh} and the thermal time constant $t_{thermal} = \rho_l c_{p,l} D_0^2 / (6 k_{g,\infty} \overline{Nu})$. The latter can be
 554 deduced from Equation 8 (see also [69]) in which the surface area variation has been omitted
 555 for simplicity. At $t=0.1t_{thermal}$ the temperature of a sphere will be $\sim 0.095(T_\infty - T_0)$, which can be
 556 a reasonable value for evaporating droplets, but still too high for droplet undergoing breakup.
 557 In any case, the ratio of these timescales ($0.1t_{thermal}/t_{sh}$) is large (see Fig. 15a), implying that the
 558 droplet heating is a much slower process relative to the droplet breakup and it becomes less
 559 significant for high We numbers and high temperatures. In a microscopic level the associated
 560 timescales are the hydrodynamic timescale $t_{hydr,liq} = R^2 / (\nu_l Re_l)$ (from [28] and Re_l from Equation
 561 13) and the heat timescale of the liquid phase $t_{heat,liq} = R^2 / a_l$, where a_l is the thermal diffusivity
 562 of the liquid phase. Their ratio is shown in Fig. 15b as a function of We number and gas phase
 563 temperature. This figure also verifies that heating plays a minor role since it is over 3 orders of
 564 magnitude slower than the momentum transport and becomes even less important for high We

565 cases. Other timescales examined based on gas phase properties and flow timescales (D/U)
 566 have shown similar trends.

567



568

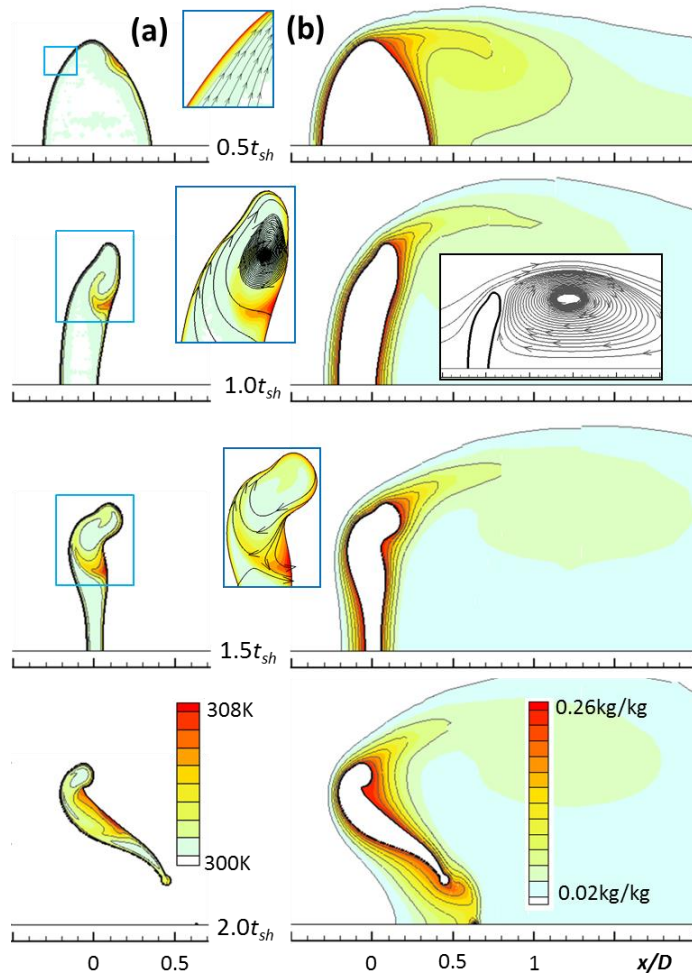
569 Fig. 15: Comparison of heating and flow timescales in (a) macroscopic and (b) microscopic
 570 level as a function of We number and gas phase temperature.

571

572 3.3.3 Spatial distribution of flow variables

573 The spatial distribution of the droplet temperature and vapour concentration is shown in Fig.
 574 16 for the case of $We=15$ and $T_{\infty}=600\text{K}$. In the front of the droplet, higher temperatures are
 575 observed due to the hot oncoming flow. A very thin thermal boundary layer can be seen on the
 576 inset figures in Fig. 16a, while at the rear of the droplet the thermal boundary layer is relatively
 577 thicker affected by the internal liquid vortex which tends to transfer hot fluid from the hotter
 578 surface towards the cooler inner droplet region. This confirms that the internal droplet
 579 temperature distribution is mainly affected by convection rather than by conduction as stated
 580 in Schlottke et al. [53]. The vapour concentration field shown in Fig. 16b is affected by the
 581 recirculation zone in the gaseous phase and higher concentration values (except of the interface
 582 region) are observed off-axis. A slightly different temperature field is observed in the high We
 583 number case of 90 at the same gas temperature, which is shown in Fig. 17a. This time, the

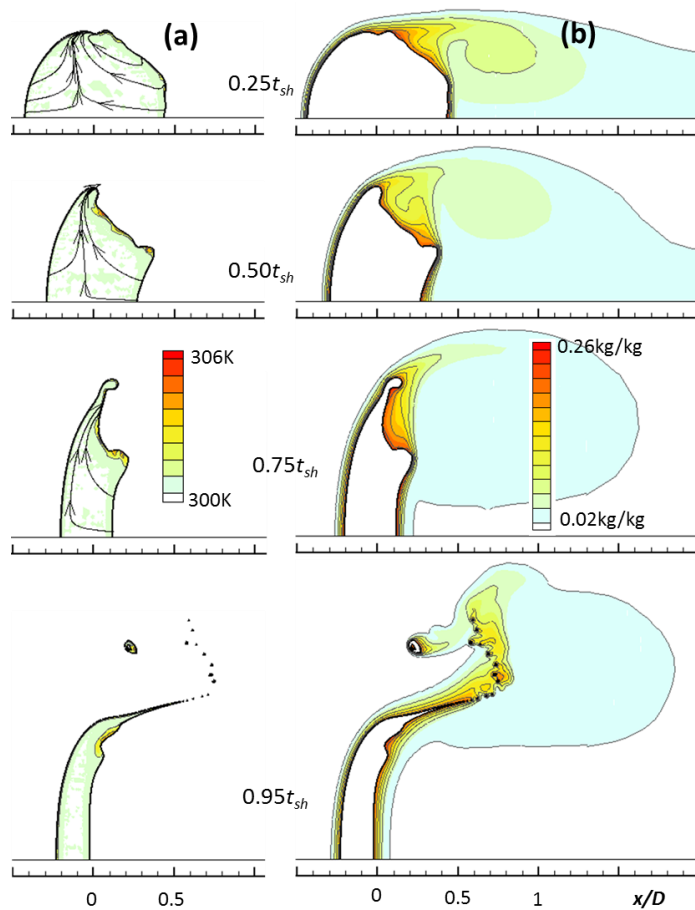
584 mixing of temperature inside the liquid phase is almost absent due to the large difference
 585 between the associated time-scales previously discussed, but also due to the fact that there are
 586 no vortices inside the droplet.



587

588 Fig. 16: Spatial distribution of (a) droplet temperature and (b) vapour concentration for the case
 589 $(We, T_\infty) = (15, 600)$. The inset figures aim to clarify the local relative velocity field.

590



591

592 Fig. 17: Spatial distribution of (a) droplet temperature along with characteristic streamlines of
 593 the relative velocity field and (b) vapour concentration for the case $(We, T_\infty) = (90, 600)$.

594

595 4 Conclusions

596 A validated numerical model, which accounts for the Navier-Stokes equations coupled with the
 597 conservation of energy and species transport equations and the VOF methodology for capturing
 598 the gas-droplet interface, has been used to study the deformation and breakup of droplets at
 599 various We and Re numbers under either isothermal or evaporating conditions. The simulations
 600 verify that the We number is the controlling parameter defining the breakup outcome. For low
 601 We numbers there is a critical Re number that controls the occurrence of breakup. The numerical
 602 results obtained under isothermal conditions are in accordance with experimental observations

603 concerning the breakup time, the droplet deformation, the droplet velocity and the drag
604 coefficient. When heating and evaporation are included, the surface tension coefficient
605 decreases due to droplet heating, but the overall hydrodynamic behaviour is not remarkably
606 changing, which is due to the short duration of the phenomenon relative to the heating timescale
607 as also to the high volatility of the fuel examined which suppresses the droplet heat-up.
608 Nevertheless, at low We numbers the associated timescales become closer and in combination
609 with the large temperature difference between liquid and gas, the critical Re number for breakup
610 becomes smaller. Relative to a spherical droplet, the increased liquid surface area due to the
611 droplet deformation enhances the droplet heating and evaporation, but the evaporated mass is
612 not exceeding 2% up to the instant of breakup.

613 By post-processing the CFD data for droplet heating and evaporation, an enhanced 0-D model
614 is derived for a simple but still accurate estimation of droplet temperature and evaporation rate
615 up to the breakup instant. Relative to classical 0-D models, the present one predicts also the
616 surface temperature and it requires the knowledge of the surface area temporal evolution.
617 Finally, the numerical predictions indicate that the spatial distribution of the vapour and
618 temperature is affected by the vortices formed within the gas and the liquid phase. This is
619 evident in the internal liquid temperature distribution for high We numbers, in which the
620 absence of internal circulation leads to trapping the hot liquid near the interface.

621

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626

627 **6 Nomenclature**

628 **Roman symbols**

Symbol	Description	Units
B	adjustable coefficient	-
B_M	Spalding number $B_M = (Y_s(T_s) - Y_\infty)/(1 - Y_s(T_s))$	-
B_T	Thermal Spalding number $B_{T,\infty} = c_{p,g,\infty}(T_\infty - T_0)/L$	-
C	Courant number $C = u \cdot \delta t / \delta x$	-
C_D	drag coefficient	-
c_p	Heat capacity	J/kgK
D	diameter	m
D_{AB}	Vapour diffusion coefficient	m ² /s
Oh	Ohnesorge number $Oh = \mu_l / \sqrt{\rho_l \sigma D_0}$	-
k	Thermal conductivity	W/mK
L	Latent heat of vaporization	J/kg
m	mass	kg
\dot{m}''	Evaporation rate per unit area	kg/m ² s
Nu	Nusselt number	-
p	pressure	Pa
Pe	Peclet number $Pe = Re \cdot Pr$	-
Pr	Prandtl number	-
R	radius	m
Re	Reynolds number $Re = \rho_g U_{rel,0} D_0 / \mu_g$	-
S	surface area	m ²
Sc	Schmidt number	-
Sh	Sherwood number	-
t	time	s
t_{sh}	Shear breakup timescale $t_{sh} = D\sqrt{\varepsilon}/U$	-
T	temperature	K
U	reference velocity	m/s
u	instantaneous droplet velocity	m/s
V	volume	m ³
We	Weber number $We = \rho_g U_{rel,0}^2 D_0 / \sigma$	-
We_t	instantaneous We number	-
X	droplet displacement	m
Y	vapour concentration	kg/kg

629

630

631 **Greek symbols**

Symbol	Description	Units
a	thermal diffusivity	m ² /s
γ	thermal effusivity $\gamma = \sqrt{k\rho c_p}$	J/m ² Ks ^{0.5}

δt	timestep	s
δx	cell size	m
ε	density ratio $\varepsilon = \rho_l / \rho_g$	-
μ	viscosity	kg/ms
N	viscosity ratio $N = \mu_l / \mu_g$	-
ν	kinematic viscosity	m ² /s
ρ	density	kg/m ³
σ	surface tension coefficient	N/m

632

Subscripts

Symbol	Description
0	initial
c	cross-stream
cr	critical
g	gas
l	liquid
rel	relative
s	at surface
t	instantaneous magnitude
x,y,z	coordinates
∞	free-stream conditions

633

Abbreviations

Symbol	Description
BFW	Body Force Weighted
BSOI	Bounded Second Order Implicit
CFD	Computational Fluid Dynamics
cpR	Cells per Radius
CSS	Continuum Surface Stress
FOU	First Order Upwind
PISO	Pressure-Implicit with Splitting of Operators
SOU	Second Order Upwind
UDF	User Defined Function

634

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636

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