



# City Research Online

## City St George's, University of London

**Citation:** Stefanitsis, D., Strotos, G., Nikolopoulos, N., Kakaras, E. & Gavaises, M. (2019). Improved droplet breakup models for spray applications. *International Journal of Heat and Fluid Flow*, 76, pp. 274-286. doi: 10.1016/j.ijheatfluidflow.2019.02.010

This is the preprint version of the paper.

This version of the publication may differ from the final published version. To cite this item please consult the publisher's version.

**Permanent repository link:** <https://openaccess.city.ac.uk/id/eprint/21813/>

**Link to published version:** <https://doi.org/10.1016/j.ijheatfluidflow.2019.02.010>

**Copyright and Reuse:** Copyright and Moral Rights remain with the author(s) and/or copyright holders. Copies of full items can be used for personal research or study, educational, or not-for-profit purposes without prior permission or charge, unless otherwise indicated, provided that the authors, title and full bibliographic details are credited, a hyperlink and/or URL is given for the original metadata page and the content is not changed in any way. For full details of reuse please refer to [City Research Online policy](#).

# Improved droplet breakup models for spray applications

## Affiliations

Dionisis Stefanitsis<sup>\*1,2</sup>, George Strotos<sup>3</sup>, Nikolaos Nikolopoulos<sup>1</sup>, Emmanouil Kakaras<sup>1</sup>, Manolis Gavaises<sup>2</sup>

<sup>1</sup>Centre for Research and Technology Hellas/Chemical Process and Energy Resources Institute (CERTH/CPERI), Egialeias 52, Marousi, Greece

<sup>2</sup>City University London, School of Engineering and Mathematical Sciences, Northampton Square, EC1V 0HB London, UK

<sup>3</sup>Technological Educational Institute of Thessaly, Mechanical Engineering Department, 41110 Larissa, Greece

\*Corresponding author: stefanitsis@certh.gr

[gstrot@teilar.gr](mailto:gstrot@teilar.gr), [n.nikolopoulos@certh.gr](mailto:n.nikolopoulos@certh.gr), [ekak@central.ntua.gr](mailto:ekak@central.ntua.gr), [M.Gavaises@city.ac.uk](mailto:M.Gavaises@city.ac.uk)

## Abstract

The current study examines the performance of two zero-dimensional (0D) aerodynamically-induced breakup models, utilized for the prediction of droplet deformation during the breakup process in the bag, multi-mode and sheet-thinning regimes. The first model investigated is an improved version of the widely used Taylor analogy breakup (TAB) model, which compared to other models has the advantage of having an analytic solution. Following, a model based on the modified Navier-Stokes (M-NS) is investigated. The parameters of both models are estimated based upon published experimental data for the bag breakup regime and CFD simulations with Diesel droplets performed as part of this work for the multi-mode and sheet-thinning regimes, for which there is a scarcity of experimental data. Both models show good accuracy in the prediction of the temporal evolution of droplet deformation in the three breakup regimes, compared to the experimental data and the CFD simulations. It is found that the best performance of the two is achieved with the M-NS model. Finally, a unified secondary breakup model is presented, which incorporates various models found in the literature, i.e. TAB, non-linear TAB (NLTAB), droplet deformation and breakup (DDB) and M-NS, into one equation using adjustable coefficients, allowing to switch among the different models.

## Keywords

droplet breakup models; droplet deformation; TAB; CFD;

## Nomenclature

### Roman symbols

$C_d$  Viscosity coefficient [-]

$C_f$  Pressure coefficient [-]

$C_k$  Surface tension coefficient [-]

$D$  Droplet diameter [m]

$E$  Energy [J]

$\alpha$  Rate of stretching [-]

$\varepsilon$  Density ratio [-]

$\mu$  Dynamic viscosity [kg/(m·s)]

$\rho$  Density [kg/m<sup>3</sup>]

$\sigma$  Surface tension [N/m]

### Subscripts/Superscripts

<i>F</i>	Force [N]	*	Non-dimensional quantity
<i>f</i>	Adjustable parameter [-]	<i>O</i>	Initial
<i>h</i>	Rim thickness [m]	cm	Center of mass
<i>k</i>	Curvature [1/m]	<i>cr</i>	Cross-stream
<i>m</i>	Mass [kg]	<i>d</i>	Droplet
<i>n</i>	Pressure exponent [-]	<i>def</i>	Deformation
<i>Oh</i>	Ohnesorge number [-]	<i>kin</i>	Kinetic
<i>p</i>	Pressure [Pa]	<i>L</i>	Liquid phase
<i>R</i>	Droplet radius [-]	<i>r</i>	Radial
<i>r</i>	Radial coordinate [m]	<i>ref</i>	Reference
<i>Re</i>	Reynolds number [-]	<i>rel</i>	Relative
<i>S</i>	Surface area [m <sup>2</sup> ]	<i>st</i>	Surface tension
<i>T</i>	Stress component [N/m <sup>2</sup> ]	<i>surf</i>	Surface
<i>t</i>	Time [s]	<i>press</i>	Pressure
<i>t<sub>sh</sub></i>	Shear breakup timescale [s]	<i>vis</i>	Viscous
<i>U, u</i>	Velocity [m/s]	<b>Abbreviations</b>	
<i>W</i>	Work [W]	<i>Bag-NS</i>	Bag Navier-Stokes
<i>y</i>	Dimensionless droplet deformation [-]	<i>BTB</i>	Bag-type-breakup
$\dot{y}$	Dimensionless deformation rate [-]	<i>DDB</i>	Droplet deformation and breakup
$\ddot{y}$	Dimensionless deformation acceleration [-]	DMTAB	Double mass Taylor analogy breakup
<i>x</i>	Axial coordinate [m]	<i>M-NS</i>	Modified Navier-Stokes
<b>Greek symbols</b>		<i>NLTAB</i>	Non-linear Taylor analogy breakup

35

## 36 1 Introduction

37 Research on liquid sprays has received a lot of attention due to their numerous applications, ranging  
38 from pharmaceutical to internal combustion engines [1]. Modeling of such systems is difficult due to  
39 the complex physical phenomena involved in them, also occurring in various time and length scales.  
40 One way to model as fast as possible such systems with acceptable accuracy, is by utilizing macroscopic  
41 CFD spray codes following the Lagrangian approach, which estimate the trajectory of each droplet as  
42 well as its deformation [2]. The former can be calculated using the drag coefficient of each droplet and  
43 the droplet motion equation. The drag coefficient of deforming droplets has been thoroughly studied  
44 in [3-17]. The droplet deformation, which is the focus of this study, is usually quantitatively described  
45 by the cross-stream droplet diameter and several models have been developed for its estimation as a  
46 function of time. These can be classified into empirical correlations based on experimental  
47 observations and semi-analytic/theoretical models, which are based on physical principles.  
48 Various studies in the literature conducted experiments of aerodynamic droplet breakup and based  
49 on their results they proposed empirical correlations for the prediction of the droplet deformation as  
50 a function of the non-dimensional time. These correlations can be written in the general form of  $y =$   
51  $c_0 + c_1(t^*)^{c_2} + c_3(t^*)^2$ , where  $y$  is the non-dimensional deformation (Figure 2), whilst the coefficients  $c_0, c_1,$   
52  $c_2$  and  $c_3$  are summarized for each study in Table 1, along with their range and conditions of

53 applicability. Apparently, these correlations perform quite well when compared against the  
 54 experimental data that they were based upon, and the question arises is if they also perform well  
 55 against other data at a) similar conditions and b) at different breakup modes. This is addressed in  
 56 Appendix A in which the model results are compared against the experimental data of [12, 18-22] in  
 57 the three main breakup regimes (bag, multi-mode and sheet-thinning) for Weber numbers in the range  
 58 of 15 to 101. In the bag breakup regime ( $We=15-20$ ) the model of Chou and Faeth [18] shows the best  
 59 agreement with the experimental data, in the multi-mode regime ( $We=52.6$ ) that of Cao et al. [23] and  
 60 in the sheet-thinning regime the model of Gel'fand et al. [24] ( $We=101$ ). None of the models is able to  
 61 accurately predict the droplet deformation in all the examined regimes.

62  
 63 Table 1. Summary of empirical correlations for droplet deformation.

<b>General equation: <math>y=c_0+c_1(t^*)^{c_2}+c_3(t^*)^2</math></b>							
Study	$c_0$	$c_1$	$c_2$	$c_3$	Conditions of applicability <sup>*1</sup>		
					Non-dimensional numbers	Breakup mode	Time range
Gel'fand et al. [24]	1	$1- We/We_{cr}$	1	0	$We=24-180$	Bag, multi-mode, sheet-thinning	$t^* \leq 1.5$
Hsiang and Faeth [20]	1	$0.23We^{1/2}$	1	0	$We=4-10^5$	Deformation up to sheet-thinning	-
Chou and Faeth [18]	1	0.5	1	0	$We=13-20,$ $Oh<0.05$	Bag	$t^* \leq 2$
	1.43	-0.18	1	0.25			$2 \leq t^* \leq 4$
	-2.51	1.79	1	0			$4 \leq t^* \leq 6$
Cao et al. [23]	1	0	0	0	$We=28-41,$ $Oh<0.003$	Multi-mode	$t^* \leq 0.3$
	0.59	1.34	1	0			$0.3 < t^* < 0.99$
Zhao et al. [25]	1	0.54	1.67	0	$We=16-26,$ $Oh<0.4$	Multi-mode	$t^* \leq 1.5$

64  
 65 <sup>1</sup>Refers to the conditions of the experiments that the corresponding model was based upon. The models are  
 66 generally valid for low  $Oh$  numbers

67  
 68 Turning now to the theoretical and semi-analytical models for the droplet deformation and breakup,  
 69 the majority of them is based on one of the two basic principles: i) conservation of momentum or ii)  
 70 conservation of energy. O'Rourke and Amsden [26] proposed the so called Taylor analogy breakup  
 71 (TAB) model in which the droplet is assumed to oscillate between its initial spherical shape and that of  
 72 the deformed oblate shape. The droplet oscillates similarly to a mass-spring-damper system with the  
 73 surface tension force being the restoring force, the viscosity representing the damping force and the  
 74 aerodynamic force being the external force acting on the droplet. Lee et al. [27] indicated later that  
 75 the TAB model shows good agreement with the experiment of Krzeczowski [22] for the breakup of a  
 76 water droplet with  $We=101$ . Later, Kim et al. [28] tuned these coefficients to match the results of their

77 experiments for Diesel droplets at  $We$  numbers in the range of 9.6 up to 26.6. Finally, Marek [29]  
78 introduced another degree of freedom to the mathematical formulation of TAB, so as to include also  
79 the translational motion of the droplet. A second mass was added to the system, which could move  
80 and oscillate independently, and thus the system resembled the system configuration of a double  
81 mass-spring-damper giving the name to the model as double mass TAB (DMTAB). The DMTAB is  
82 applicable to the deformation and bag breakup regimes and its advantage over the TAB model is that  
83 it can treat cases with low density ratios ( $\epsilon$ ) and high  $Oh$  numbers in which the droplet translational  
84 velocity changes significantly.

85 Another approach on breakup models still based on the momentum balance, is that of Villermaux and  
86 Bossa [30], in which they utilized the inviscid Navier-Stokes equations in cylindrical coordinates for the  
87 liquid droplet and the quasi-steady conservation of momentum and mass for the gas phase, to  
88 estimate the temporal variation of the droplet deformation in the bag breakup regime. Opfer et al.  
89 [31] used the momentum balance on the droplet as well, which was approximated by a cylinder of the  
90 same radius, to predict the droplet deformation in the bag breakup regime. Later, Kulkarni and Sojka  
91 [19] added the effect of viscosity to the model of [30] and it showed good agreement with their own  
92 experimental data for  $We$  numbers ranging from 13 up to 15.

93 Instead of utilizing the momentum balance on the droplet, Detkovskii and Frolov [32] and later Wang  
94 et al. [33, 34] utilized the equation of the linear strain of the droplet along its cross-stream axis to  
95 estimate the droplet deformation. They called the model BTB (bag-type breakup) and its results  
96 showed good agreement against the experimental data of [18, 22] in the bag breakup regime.

97 Regarding the theoretical models based on the conservation of energy, Ibrahim et al. [35] developed  
98 the so called deformation and breakup model (DDB), which is applicable to deforming droplets for  $We$   
99 numbers greater than 20. Rimbart et al. [36] improved the DDB model by assuming potential flow  
100 around the droplet and extensional flow (i.e. with no shear) inside the droplet. The resulting model  
101 showed acceptable agreement with the experimental data of [22, 31] for  $We$  numbers equal to 11.5,  
102 18.4 and 103.5, while the agreement was not good for the case of  $We=13.5$ . Schmehl and co-workers  
103 [37, 38] utilized the mechanical energy balance on the droplet to derive a non-linear differential  
104 equation similar to that of TAB, which they named non-linear TAB (NLTAB). This equation accounts for  
105 the modification of the aerodynamic forces imposed by the deformation of the droplet, and it showed  
106 good agreement with the experimental data of [21, 39] for the time variation of droplet deformation.

107 Finally, Sichani and Emami [40] utilized the virtual work principle to describe the droplet deformation  
108 in the deformation and bag breakup regimes. The results of the model showed good agreement with  
109 the experimental data of [18, 21, 22, 41, 42] for  $We$  numbers ranging from 12.5 up to 20.

110 The aforementioned theoretical models are summarized in Table 2 along with their basic  
111 characteristics. In addition, the performance of selected models (TAB, DDB, NLTAB, Rimbart et al. [36]  
112 and Kulkarni and Sojka [19]) is evaluated by comparing their results with the experimental data of [12,  
113 18-22] in the three breakup regimes (bag, multi-mode and sheet-thinning) for  $We=15-101$ , as  
114 presented in Appendix A. For  $We=15$  the model of Kulkarni and Sojka [19] agrees well with the  
115 experimental data, while for  $We=52.6$  and  $We=110$  the DDB model gives the best results overall. For  
116  $We=20$  all models deviate from the experimental data. Similar to the empirical models, none of the

117 examined theoretical models is able to accurately predict the droplet deformation in all the examined  
 118 regimes.

119

120

Table 2. Summary of theoretical and semi-analytical models for droplet breakup.

Model	Basic principle	Droplet shape	Pressure distribution around the droplet	Internal circulation	Coupling with translational motion	Breakup condition	Adjustable parameters	Applicability *1
TAB [43]	Momentum conservation	Ellipsoid	Uniform	No	No	$y_c=2$	3	-
NLTAB [37, 38]	Energy balance	Ellipsoid	Spatial	Yes	No	$y_c=1.8$ and $\dot{y}=0$ or $y_c=2.1$	1	-
DMTAB [29]	Momentum conservation	Ellipsoid	Uniform	No	Yes	$y_c=2$	3	$We \leq 50$ , large and small $\epsilon$ and $Oh$
DDB [35]	Energy balance	Ellipsoid (planar)	Uniform	No	No	$y_c=(We/2)/(6\pi)$	0	$We > 20$
Rimbert et al. [36]	Energy balance	Ellipsoid	Spatial (potential flow)	Yes (homotetical deformation)	Yes	$y_c=2$	0	-
BTB [32-34]	Linear strain equation	Ellipsoid	Uniform	No	No	$(B^{-1}+B^5-2B^{-4})/30 > We$ , $B=(3\pi/4)y$	1	$10 < We < 35$ , $Oh < 0.1$
Opfer et al. [31]	Momentum conservation	Cylinder	Spatial (parabolic)	No	No	-	2	$11 < We < 25$
Kulkarni and Sojka [19]	Momentum and mass conservation (Navier-Stokes)	Bag	Spatial (stagnation point)	No	No	-	1	$12 < We < 16$
Sichani and	Lagrange-type equation	Bag	Spatial	Yes	No	$\frac{4}{3} \frac{1-K}{y_1^2+y_2^2}^{*2}$	1	$We \leq 20$ , $Re > 100$ , $\epsilon > 500$ ,

121

122 <sup>1</sup>Applicability is based on the original paper proposing the model.

123 <sup>2</sup> $K$  is a parameter;  $y_1$  and  $y_2$  are the deformations in both axes.

124

125 The aforementioned observations lead to the conclusion that there is a lack of a single accurate enough  
126 model for the prediction of droplet deformation for a wide range of  $We$  numbers in the three basic  
127 breakup regimes: i) bag, ii) multi-mode and iii) sheet-thinning. So far, the TAB model is widely used in  
128 spray codes due to its simplicity, since it has an analytic solution. Nevertheless, it predicts oscillatory  
129 deformation, which is not realistic. On the other hand, the recently developed model of Kulkarni and  
130 Sojka [19] (termed as bag-Navier-Stokes or bag-NS for the remaining of the paper) predicts an  
131 exponential growth, which agrees well with experimental observations for the bag breakup mode, but  
132 it cannot be used to other breakup modes. The scope of the present work is to extend these two  
133 models.

134 Regarding the TAB model, its coefficients are re-estimated to match the actual deformation, whilst the  
135 bag-NS is modified so it can be extended to other breakup modes and is termed as M-NS (modified  
136 Navier-Stokes). The parameters of both models are specified in each breakup regime, based both on  
137 experimental data available in the literature ( $We=15-20$ ) and CFD simulations performed as part of this  
138 study ( $We=20-350$ ). Finally, in Appendix B several breakup models (TAB, DDB, NLTAB and NS) are  
139 presented in a unified way using a common equation along with adjustable coefficients to switch to  
140 the different models (termed as unified secondary breakup model). It should be mentioned that this  
141 work focuses only on the effect of  $We$  number, while a sperate investigation is required for the effect  
142 of other non-dimensional numbers ( $Oh$ ,  $\varepsilon$ ,  $Re$ ) as well as the effect of ambient temperature.

143 In the following sections, initially the computational setup and examined conditions of the CFD  
144 simulations are presented, followed by the description of the mathematical models of the TAB and M-  
145 NS models. It follows the presentation of the results of each model along with experimental data and  
146 the results of the CFD simulations. Finally, the conclusions and recommendations are summarized in  
147 the last section of the paper.

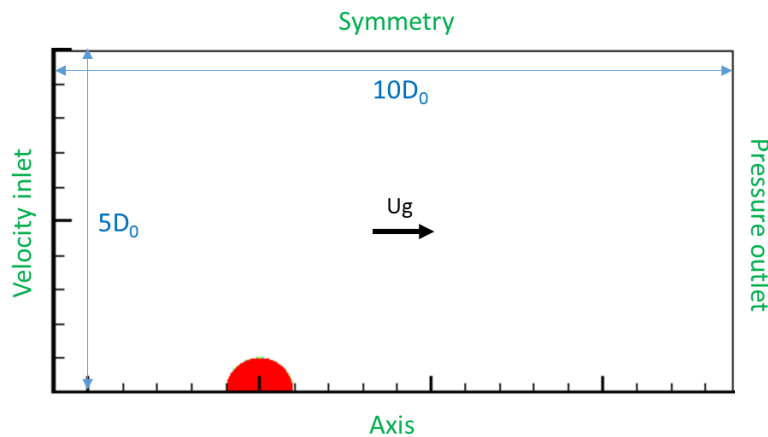
148

## 149 **2 Computational setup and examined conditions**

150 Apart from utilizing experimental data for the estimation of the model parameters, complimentary  
151 CFD simulations have also been performed. The CFD simulations are utilized for the derivation of the  
152 parameters of the improved TAB and M-NS models in the multi-mode and sheet-thinning regimes, in  
153 which there is a scarcity of experimental data to cover substantially the whole range of  $We$  numbers  
154 ( $We=21-350$ ). In addition, the simulations provide useful information regarding the critical  
155 deformation, which is necessary for the extraction of a breakup condition that is utilized in both  
156 breakup models.

157 The numerical CFD model solves the Navier-Stokes equations coupled with the Volume of Fluid (VOF)  
158 methodology [44] for tracking the interface between the liquid droplet and the surrounding gas. The  
159 surface tension forces are modelled with the Continuum Surface Stress (CSS) model of [45]. The  
160 simulations are performed in a two-dimensional axisymmetric domain with the commercial CFD tool

161 ANSYS FLUENT v16 [46]. At low Reynolds numbers, such as those examined in this work (Table 4), the  
 162 axisymmetric approximation has proven to be relatively accurate during the deformation stages of  
 163 breakup [16, 47, 48]. Various User Defined Functions (UDFs) are employed for i) the adaptive local grid  
 164 refinement technique around the liquid-gas interface [49], ii) the adaptive time-step scheme for the  
 165 implicit VOF solver based on the velocity at the droplet interface [13], and iii) the moving mesh  
 166 technique based on the average velocity of the droplet. The CFD model has been developed and  
 167 validated in previous works for the case of aerodynamic droplet breakup [13, 16, 17, 50-53], as well as  
 168 for other applications such as the free fall of droplet [49], the droplet impingement on a flat wall [54]  
 169 or a spherical particle [55-57], and the droplet evaporation [13, 52, 58].  
 170 The 2-dimensional axisymmetric computational domain and boundary conditions are presented in  
 171 Figure 1. The droplet is initially stagnant, while air flows from the left boundary with a constant velocity  
 172  $U_g$ , causing it to move and deform. The computational cells have a rectangular shape with a base grid  
 173 resolution equal to  $3cpR$  (cells per radius), while 6 levels of local grid refinement are applied to obtain  
 174 the desired resolution of  $192cpR$  around the liquid-gas interface. The resolution of  $192cpR$  is adequate  
 175 for the simulations of droplet breakup, since simulations with 48, 96, 192 and 384cpR have shown that  
 176 the average drop velocity and deformation change less than 1% when a finer grid is used.  
 177



178  
 179 Figure 1. Computational domain and boundary conditions for the CFD simulations.  
 180

181 The liquid properties correspond to those of Diesel fuel, while the surrounding gas is air at  $T=293.15K$   
 182 and  $P=1bar$  (energy equation not solved). Although Diesel is utilized as test fuel in the current work,  
 183 the results can be considered valid for low viscosity fuels as long as the Ohnesorge number is kept  
 184 below 0.1 [59]. The same is true for the effect of ambient pressure or equivalently that of the density  
 185 ratio, which becomes important approximately below 32 [53, 60]. Both the properties of Diesel and air  
 186 as well as the droplet diameter are based on [61] as presented in Table 3. The corresponding non-  
 187 dimensional numbers are  $\epsilon=678$ ,  $Oh=0.038$  and  $N=117$  (eq. (3)). The high density ratio ( $\epsilon$ ) and low  $Oh$   
 188 number ensure that their effect is minimized, focusing only on the effect of  $We$  number. By altering  
 189 the gas velocity, the resulting  $We$  numbers range from 20 up to 350, resulting in 21 simulations in the  
 190 three breakup regimes, i.e. those of bag, multi-mode and sheet-thinning, as shown in Table 4. The  
 191 corresponding  $Re$  numbers range from 531 to 2221.  
 192

193

Table 3. Properties of liquid Diesel and air at  $T=293.15\text{K}$  and  $P=1\text{bar}$  based on [61].

$D_0$ ( $\mu\text{m}$ )	$P$ (bar)	$T_g$ (K)	$\mu_g$ (kg/s·m)	$\rho_g$ (kg/m <sup>3</sup> )	$T_L$ (K)	$\mu_L$ (kg/m·s)	$\rho_L$ (kg/m <sup>3</sup> )	$\sigma$ (N/m)
198	1	293.15	1.85E-05	1.215	293.15	0.00217	824	0.02

194

195

Table 4. Examined cases of CFD simulations.

Case	$U_{g,0}$ (m/s)	$We$	$Re$	$Oh$	$\varepsilon$	$N$
1	40.8	20	531	0.038	678	117
2	43.7	23	569	0.038	678	117
3	49.1	29	639	0.038	678	117
4	53.2	34	692	0.038	678	117
5	57.7	40	751	0.038	678	117
6	64.5	50	839	0.038	678	117
7	67.6	55	880	0.038	678	117
8	70.6	60	920	0.038	678	117
9	76.3	70	993	0.038	678	117
10	81.5	80	1062	0.038	678	117
11	86.5	90	1126	0.038	678	117
12	91.2	100	1187	0.038	678	117
13	95.6	110	1245	0.038	678	117
14	99.9	120	1300	0.038	678	117
15	103.9	130	1354	0.038	678	117
16	107.9	140	1405	0.038	678	117
17	111.7	150	1454	0.038	678	117
18	128.9	200	1679	0.038	678	117
19	144.1	250	1877	0.038	678	117
20	157.9	300	2056	0.038	678	117
21	170.6	350	2221	0.038	678	117

196

### 197 3 Mathematical model

#### 198 3.1 Non-dimensional numbers

199 The non-dimensional numbers that are commonly used to describe the breakup of isolated droplets  
 200 are the Weber ( $We$ ), Ohnesorge ( $Oh$ ) and Reynolds ( $Re$ ) numbers as well as the density ( $\varepsilon$ ) and viscosity  
 201 ratios ( $N$ ) of the two phases [59].

202

$$202 \quad We = \frac{\rho_g U_0^2 D_0}{\sigma} \quad Oh = \frac{\mu_L}{\sqrt{\rho_L \sigma D_0}} \quad Re = \frac{\rho_g U_0 D_0}{\mu_g} \quad \varepsilon = \frac{\rho_L}{\rho_g} \quad N = \frac{\mu_L}{\mu_g} \quad (1)$$

203

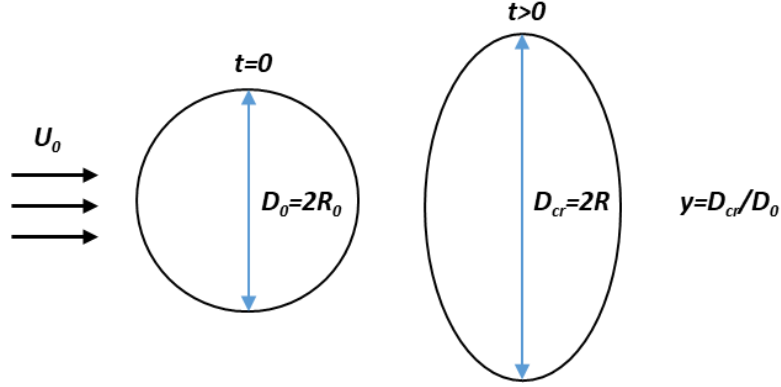
204 The breakup timescale proposed by Nicholls and Ranger [62] is used as a convenient non-  
 205 dimensionalisation parameter for time ( $t^*=t/t_{sh}$ ):

206

$$206 \quad t_{sh} = \frac{D_0}{U_0} \sqrt{\varepsilon} \quad (2)$$

207  
208  
209  
210  
211

Finally, the non-dimensional droplet deformation ( $y$ ), which is the quantity of most importance in this work, is quantitatively described by the non-dimensional cross-stream diameter of the droplet ( $D_{cr}/D_0$ ), as shown in Figure 2.



212  
213  
214

Figure 2. Definition of the cross-stream droplet diameter and the non-dimensional droplet deformation.

### 3.2 Improved TAB model

O'Rourke and Amsden [43] derived the differential equation of the TAB model for the displacement of the drop equator compared to that of a spherical shape. By introducing the non-dimensional droplet deformation ( $y$ ) and time ( $t^*$ ), as well as the  $We$  and  $Oh$  numbers the equation becomes:

$$\ddot{y} + 4C_d \frac{Oh}{\sqrt{We}} \dot{y} + \frac{8C_k}{We} (y - 1) = 4C_F \quad (3)$$

220

where  $\dot{y} = dy/dt^*$  is the dimensionless deformation rate and  $\ddot{y} = d^2y/dt^{*2}$  the dimensionless deformation acceleration.

The parameters of the improved TAB model ( $C_k$  and  $C_f$ ) are found by fitting to the results for the temporal evolution of droplet deformation of a) the experimental studies of [12, 18-21] (bag regime) and b) the results of the CFD simulations (multi-mode and sheet-thinning regimes), as presented in Table 5 along with those of the original TAB of [26]. The value of zero for the surface tension term  $C_k$  was found to fit better to the aforementioned group of results for  $We \geq 60$ , something that results in the negation of the surface tension term in the modified TAB model (eq. (3)). Thus, its solution for the droplet deformation results in an exponential function of time instead of an oscillation. The physical interpretation of this, is that for high  $We$  numbers the aerodynamic forces are much higher than the surface tension forces, and therefore the latter can be neglected. Finally, the value of the viscosity parameter  $C_d$  is taken constant and equal to 10, in agreement with [29, 63]; this parameter is expected to be a function of  $Oh$  number, which has a constant low value throughout this study and has a minor effect on the breakup process.

235  
236

Table 5. Parameters of the original and improved TAB models.

Breakup mode	Original TAB			Improved TAB		
	$C_d$	$C_f$	$C_k$	$C_d$	$C_f$	$C_k$
Bag				10	$0.13 + 0.0026We$	$-1.32 + 0.12We$
Multi-mode	5	1/3	8	10	$0.46 + 0.0022We$	$7.87 - 0.13We, We < 60$
Sheet-thinning						$0, We \geq 60$

237

### 238 3.3 Modified Navier-Stokes (M-NS) model

239 In this work we introduce a numerical improvement of the bag-NS breakup model, which has been  
240 developed in [19]; however, its derivation is repeated in Appendix C due to an erroneous calculation,  
241 which is corrected in this work. This is the multiplier of the viscosity term (2<sup>nd</sup> term from the left of eq.  
242 (28)), which is found equal to 16 in this work, while in [19] it was estimated equal to 8, probably due  
243 to a miscalculation in the algebraic manipulations. Either way, the contribution of this term in the  
244 calculation of the droplet deformation is low for the current examined conditions of low  $Oh$  numbers  
245 ( $Oh < 0.04$ ) and thus it is not affecting the results. However, its contribution is expected to increase for  
246 higher  $Oh$  numbers.

247 In the M-NS model the droplet deformation is described by equation (4). The difference with the  
248 original bag-NS model lies in the estimation of the pressure term, which is a function of  $y^n$  instead of  $y$   
249 (4<sup>th</sup> term from the left of eq. (4)). Eq. (4) is a second-order non-linear differential equation with no  
250 analytical solution, the numerical solution of which is obtained in this work using an explicit 4<sup>th</sup> order  
251 Runge-Kutta method [64, 65].

252

$$\ddot{y} + 16 \frac{Oh}{\sqrt{We}} \frac{1}{y^2} \dot{y} + \frac{24}{We} y - \frac{a^2}{4} y^n = 0 \quad (4)$$

253

254 The parameter  $a$  is called rate of stretching, while the parameter  $n$  is called pressure exponent and has  
255 been introduced in the present work to provide a more flexible numerical consideration of the  
256 pressure contribution. For  $n \geq 1$  the deformation grows exponentially in time (note that  $n=1$   
257 corresponds to the original model of [19], as shown in Table 6), while for  $n < 1$  the deformation becomes  
258 oscillatory. More specifically, for  $n=0$  the equation becomes similar to that of the TAB model, while for  
259  $n=-1$  it becomes similar to that of the NLTAB, since the pressure term is proportional to  $1/y$ . For each  
260 breakup mode, the value of  $n$  that gives the higher coefficient of determination ( $R^2$ ) is selected,  
261 compared to the results of the experimental studies of [12, 18-21] (bag regime) and the CFD  
262 simulations (multi-mode and sheet-thinning regimes), as shown in Table 6.

263 Finally, instead of using a constant value for the parameter  $a$ , the current study proposes this to be a  
264 function of the  $We$  number for each breakup mode (bag, multi-mode and sheet-thinning), as presented  
265 in Table 6. For the bag breakup regime, the experimental data of [12, 18-21] for the temporal evolution  
266 of droplet deformation are utilized, while for the multi-mode and sheet-thinning regimes the results  
267 of the CFD simulation are employed instead;  $a$  is found for each  $We$  number by fitting eq. (4) to the  
268 results and by assuming a linear dependence of  $a$  on the  $We$  number. It should be mentioned that the  
269 equation of  $a$  in the bag breakup regime gives a value of  $a$  equal to 2.88 for  $We=15$ , which is close to  
270 the value of 2.83 proposed by [19] for the same  $We$  (Table 6).

271  
272

Table 6. Parameters of the bag-NS and M-NS models.

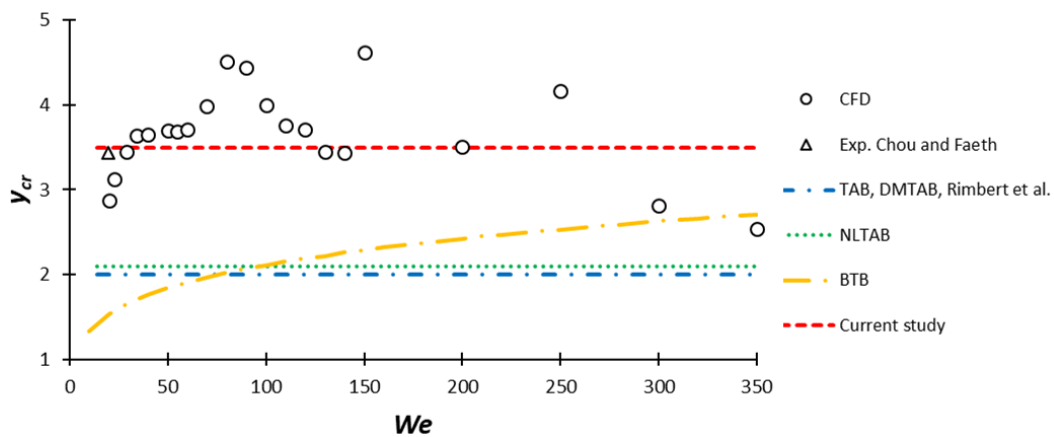
Breakup mode	Original bag-NS		Proposed M-NS	
	n	$\alpha$	n	$\alpha$
Bag	1	2.83	1	$3.6 - 0.048We$
Multi-mode	-	-	-0.5	$3.35 + 0.0032We$
Sheet-thinning	-	-	2	$2.35 + 0.0042We$

273

### 274 3.4 Breakup condition

275 Most breakup models of the literature assume a constant critical deformation (onset of breakup) in  
 276 the range of 1.8 to 2.1 (see Table 2), with the exception of the BTB model in which the critical  
 277 deformation is a function of  $We$ . In this study we assume that the breakup occurs when either the  
 278 maximum deformation is reached ( $\dot{y}=0$ ) or when a critical deformation is exceeded ( $y_{cr}=3.5$ ), whichever  
 279 comes first. The condition of  $y_{cr}=3.5$  is calculated based on the results of the CFD simulations for a  
 280 range of  $We$  numbers from 20 up to 350 and it is also in agreement with the experimental data of [18]  
 281 for a  $We$  number equal to 20, as shown in Figure 3. The critical deformation of the various models of  
 282 the literature is presented in the figure as well.

283



284

285 Figure 3. Critical deformation as estimated by the CFD simulations and the experiments of [18], as well as the  
 286 assumptions of the various breakup models.

287

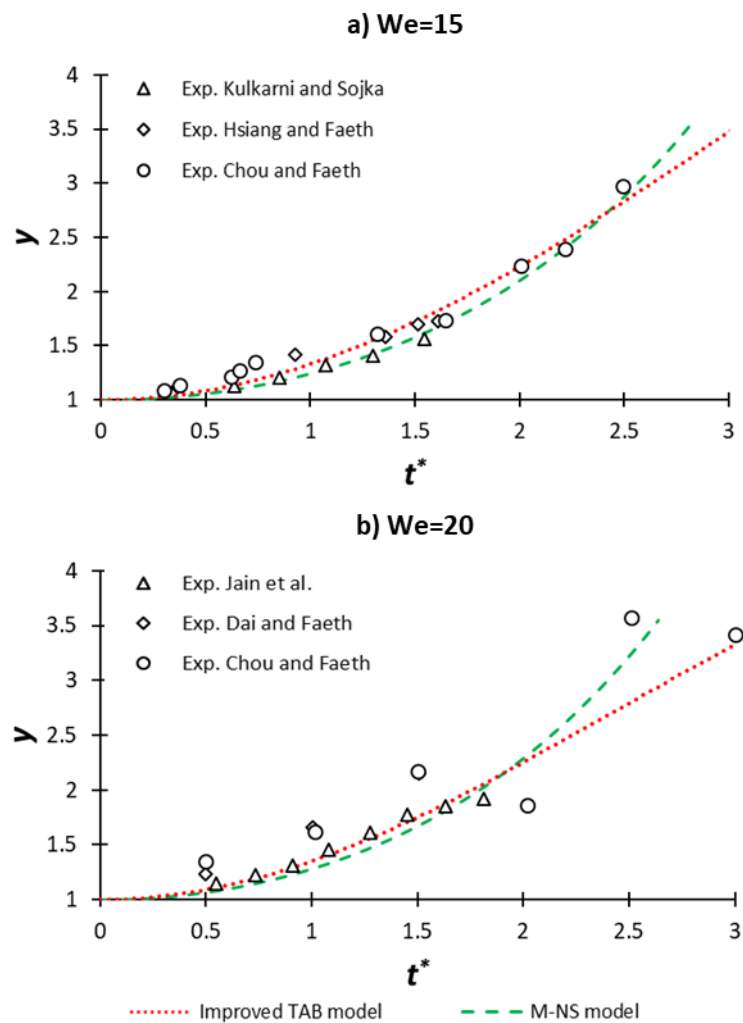
## 288 4 Results and discussion

289 The temporal evolution of droplet deformation can be calculated using the two models (improved TAB  
 290 and M-NS) with their respective equations and parameters: i) improved TAB model using eq. (3) and  
 291 the parameters of Table 5 and ii) M-NS model using eq. (4) and the parameters of Table 6. The results  
 292 are presented in the following sub-sections as calculated by the two models in the bag, multi-mode  
 293 and sheet-thinning regimes, against the results of experimental studies (bag breakup regime) and  
 294 those of the CFD simulations (multi-mode and sheet-thinning regimes).

295

### 296 4.1 Bag breakup regime - $We=10-20$

297 The results of two breakup models (improved TAB and M-NS) are illustrated in Figure 4 for two  $We$   
 298 numbers in the bag breakup regime ( $We=15$  and  $20$ ), along with those of the experimental studies for  
 299 the same  $We$  numbers [12, 18-21]. It should be noted that the experiment of Chou and Faeth [18] show  
 300 some discrepancies for the case of  $We=20$  and at  $t^*>1.5$ , since  $y$  decreases over time, something that  
 301 is not realistic. Nevertheless, they have been included both in the graph and in the fitting procedure  
 302 since they are the only data available for  $We=20$  and  $t^*>1.5$ . Both models show a good agreement with  
 303 the experimental data for both  $We$  numbers. The TAB model predicts lower values for the deformation  
 304 compared to the M-NS model at higher  $t^*(\geq 2.5)$ , owing to the assumption that the droplet deformation  
 305 is modeled as an oscillation in the TAB model, in comparison with the exponential behavior predicted  
 306 by the M-NS model.  
 307



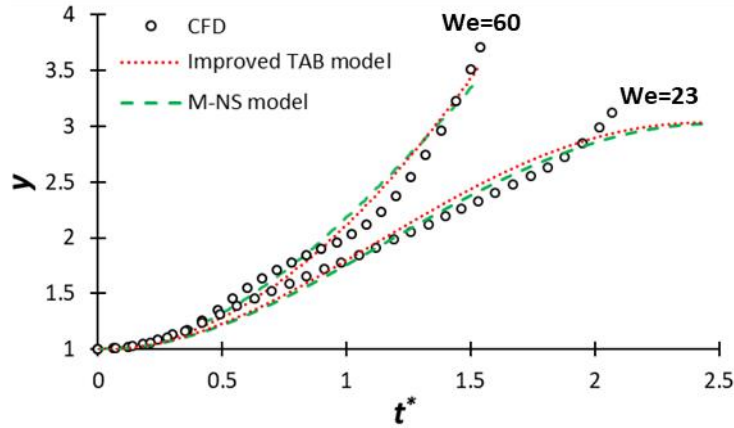
308

309 Figure 4. Temporal evolution of droplet deformation as predicted by the improved TAB and M-NS models  
 310 along with the experimental data from the literature for a)  $We=15$  and b)  $We=20$ .  
 311

#### 312 4.2 Multi-mode breakup regime - $We=21-65$

313 The results of the two breakup models are presented in Figure 5 for two  $We$  numbers, 23 and 60, in  
 314 the multi-mode regime, along with those of the simulations for the same  $We$  numbers. The agreement

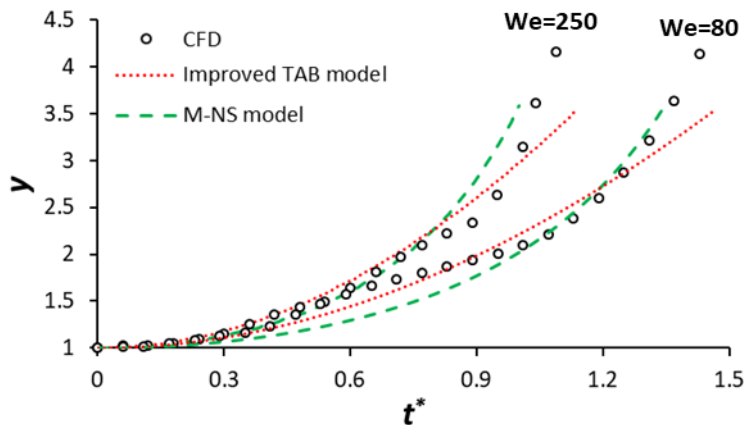
315 is good between the models and the simulations, apart from the prediction of a slightly higher breakup  
 316 initiation time for the case of  $We=23$ . This is attributed to the oscillatory behavior of the models and  
 317 the consequent occurrence of breakup at the time when  $\dot{y}=0$  and not at  $y_{cr}=3.5$ . Note that a selection  
 318 of an exponential solution for the M-NS model (parameter  $n \geq 1$ ), although it gives slightly better results  
 319 for the case of  $We=60$ , it does not agree will with the simulations for the case of  $We=23$ , and therefore  
 320 is not selected.  
 321



322  
 323 Figure 5. Temporal evolution of droplet deformation as predicted by the improved TAB and M-NS models with  
 324 the results of the simulations for two  $We$  numbers in the multi-mode regime (60 and 23).  
 325

326 **4.3 Sheet-thinning breakup regime -  $We=66-350$**

327 In Figure 6 the results from the two breakup models are presented for two  $We$  numbers (80 and 250)  
 328 in the sheet-thinning regime, along with those of the simulations for the same  $We$  numbers. Good  
 329 agreement is observed again for both models, although a slight underestimation of  $y_{cr}$  is noticed for  
 330 both  $We$  numbers, due to the higher value of  $y_{cr}$  as predicted by the simulations in the current regime.  
 331 In addition, the results of the M-NS model are closer to those of the simulations due to their steeper  
 332 inclination.  
 333



334  
 335 Figure 6. Temporal evolution of droplet deformation as predicted by the improved TAB and M-NS models  
 336 along with the results of the simulations for two  $We$  numbers in the sheet-thinning regime (80 and 250).

337

## 338 **5 Conclusions and future work**

339 The present work examined the droplet deformation and breakup models for the three basic regimes  
340 of droplet breakup, i.e. the bag, multi-mode and sheet-thinning. The publicly available empirical  
341 models of [18, 20, 23, 24] were examined as well as the theoretical models TAB, DDB, NLTAB, Rimbart  
342 et al. [36] and bag-NS [19], for their range of validity against available experimental data ( $We=15-101$ ).  
343 It was found (see Appendix A) that none of them was capable of accurately predicting the droplet  
344 deformation in all the three breakup regimes. For this reason, two existing models were improved and  
345 modified, namely i) an improved TAB model and ii) the M-NS model, which is a modified version of an  
346 existing model based on the Navier-Stokes equations.

347 The parameters of both models were estimated for each breakup regime, based both on experimental  
348 data found in the literature (bag regime) and CFD simulations with Diesel droplets performed as part  
349 of this study in the multi-mode and sheet-thinning breakup regimes, for which available experimental  
350 data are not enough to cover the entire range of values for the necessary parameters. In addition, a  
351 breakup condition was introduced ( $\dot{\gamma}=0$  or  $\gamma_{cr}=3.5$ ) based on the results of the CFD simulations and  
352 those of the experiments, which gives acceptable results for all examined cases.

353 Regarding the prediction of droplet deformation, both models showed a good agreement against the  
354 experimental data in the bag breakup regime and the CFD simulations in the multi-mode and sheet-  
355 thinning regimes, with the M-NS model showing the best performance overall.

356 It should be noted that the proposed parameters and breakup conditions for both models are valid for  
357 low  $Oh$  (low viscosity fuels), high  $\varepsilon$  and for isolated droplets, and thus a separate investigation is  
358 required for the estimation of the parameters at different conditions. Finally, a unified secondary  
359 breakup model is introduced, which consolidates into a single equations various models of the  
360 literature (TAB, NLTAB, DDB and NS), by using adjustable coefficients (see Appendix B). As a future  
361 work, the parameters of this model can be estimated based on CFD simulations, which in return may  
362 result in the formulation of a completely new deformation and breakup model.

363

## 364 **Acknowledgements**

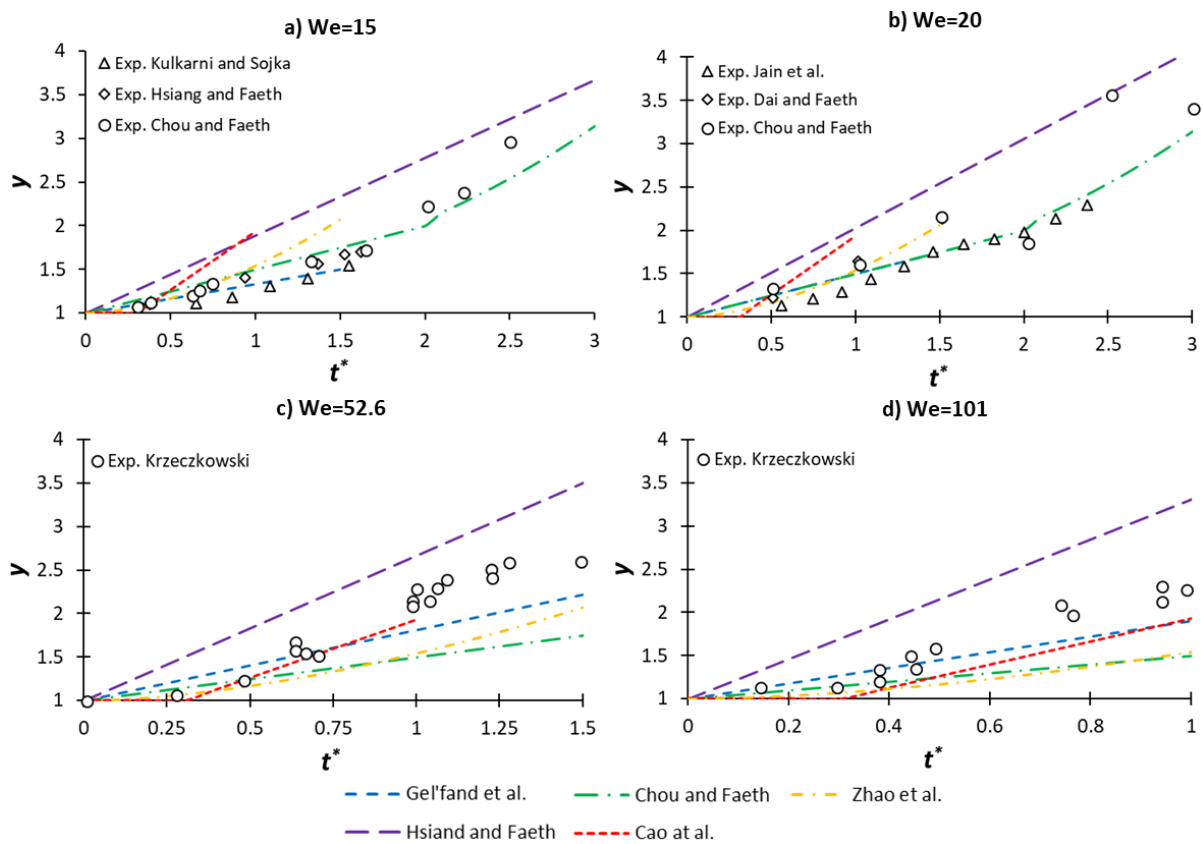
365 Financial support from the MSCA-ITN-ETN of the European Union's H2020 programme, under REA  
366 grant agreement n. 675676 is acknowledged.

367

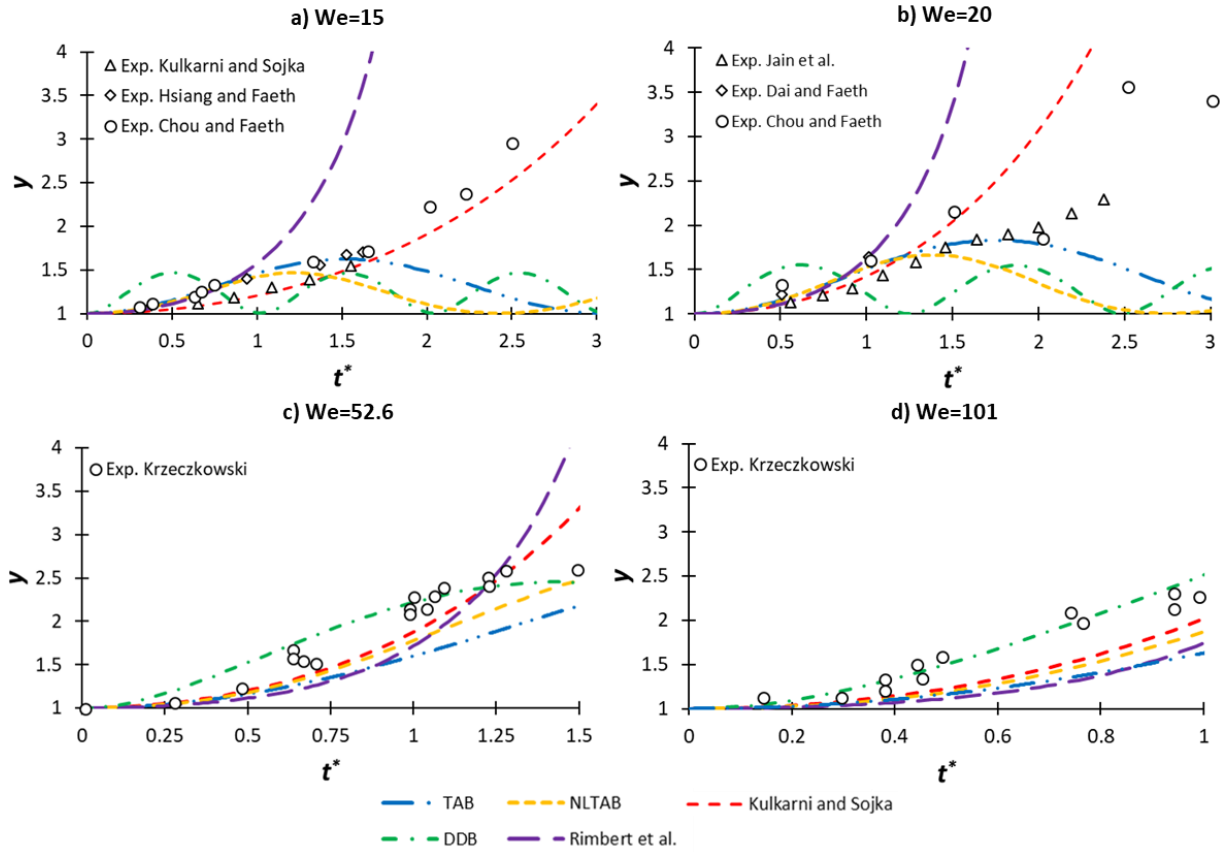
## 368 **Appendix A. Comparison of the existing deformation and breakup models with** 369 **experimental data.**

370 The temporal evolution of droplet deformation as predicted by the various models of Table 1 and  
371 selected models of Table 2 are presented in Figure 7 and Figure 8, respectively, along with various  
372 experimental data found in the literature in three breakup regimes (bag, multi-mode and sheet-  
373 thinning) for  $We=15$  [18-20],  $We=20$  [12, 18, 21],  $We=52.6$  [22] and  $We=101$  [22]. It should be noted  
374 that the applicability of some models has been extended beyond the range presented in Table 1 and  
375 Table 2 in order to assess if their range of applicability can be extended. The experiments are plotted  
376 up to the breakup initiation time, while those by [22] have been shifted in terms of time based on the  
377 results of CFD simulations at the same conditions. In the bag breakup regime ( $We=15-20$ ) the empirical

378 model of Chou and Faeth [18] and the theoretical model of Kulkarni and Sojka [19] show the best  
 379 agreement, in the multi-mode regime ( $We=52.6$ ) that of Cao et al. [23] and the DDB, and in the sheet-  
 380 thinning regime ( $We=101$ ) that of Gel'fand et al. [24] and the DDB again.  
 381



382  
 383 Figure 7. Comparison between experimental data and the predictions of the various empirical models for the  
 384 temporal evolution of droplet deformation for a)  $We=15$ , b)  $We=20$ , c)  $We=52.6$  and d)  $We=101$ .  
 385



386

387 Figure 8. Comparison between experimental data and the predictions of the various theoretical models for the  
 388 temporal evolution of droplet deformation for a)  $We=15$ , b)  $We=20$ , c)  $We=52.6$  and d)  $We=101$ .

389

### 390 Appendix B. Unified secondary breakup model.

391 In order to develop the unified secondary breakup model, a similar procedure to that of Schmehl et al.  
 392 [37] for the derivation of the NLTAB model is followed, but the appearing terms are expressed in a  
 393 more generic way. This is accomplished by utilizing basic equations, (e.g. the work is given by the  
 394 multiplication of a force with an area), along with reference values for these variables (e.g. reference  
 395 force and area). In addition, adjustable parameters are introduced to account for the effects of physical  
 396 parameters/mechanisms that are not included in the equations, since they are expressed by using  
 397 reference magnitudes, such as the internal flow in the droplet and the pressure distribution around it.  
 398 For convenience the mechanical energy balance of the droplet is employed first, which is written in  
 399 rate form in eq. (5):

400

$$\frac{dE_d}{dt} = \dot{W}_g - \dot{W}_{vis,d} \quad (5)$$

401

402 The droplet energy consists of three parts, i.e. a) the kinetic translational energy, b) the surface energy  
 403 and c) the kinetic energy as the droplet deforms. It should be noted also that heat transfer effects  
 404 could be also added in eq. (5), which are not within the scope of the current work and therefore are  
 405 neglected. It is mathematically proved that the translational droplet energy cancels the work of

406 pressure forces in the direction of the flow, using the droplet momentum equation in the streamwise  
 407 direction. Thus, the translational terms will not be included.

408 Starting with the kinetic energy this can be calculated as:

409

$$E_{kin,d} = f_{kin} \frac{1}{2} m_L U_{def,y}^2 = f_{kin} \frac{1}{2} \rho_L \frac{\pi D_0^3}{6} \left( \frac{dR}{dt} \right)^2 \quad (6)$$

410

411 The term  $U_{def,y}=dR/dt$  denotes the deformation velocity in the cross-stream direction and serves as a  
 412 scaling velocity for the calculation of the kinetic energy, while the coefficient  $f_{kin}$  is used to include the  
 413 secondary effects appearing during droplet deformation. These are: i) the secondary kinetic energy  
 414 arising from the axial (transverse) deformation, ii) the variation of liquid velocity along the cross-  
 415 stream diameter (it is 0 at the symmetry axis and  $dR/dt$  at the peripheral tip), and iii) the internal liquid  
 416 flow/circulation. In the TAB and DDB models the value of  $f_{kin}$  is equal to 1, while in the NLTAB it is a  
 417 decreasing function of  $y$  (see Table 7).

418 The rate of kinetic energy is:

419

$$\frac{dE_{kin,d}}{dt} = \frac{1}{2} \rho_L \frac{\pi D_0^3}{6} \left( f_{kin} 2 \frac{dR}{dt} \frac{d^2R}{dt^2} + \frac{df_{kin}}{dR} \left( \frac{dR}{dt} \right)^3 \right) \quad (7)$$

420

421 And by introducing the non-dimensional numbers:  $y = \frac{2R}{D_0} \rightarrow R = y \frac{D_0}{2}$  (see Figure 2) and  $t^* =$

422  $\frac{t}{D_0 \sqrt{\varepsilon}} U_0 \rightarrow t = t^* \frac{D_0 \sqrt{\varepsilon}}{U_0}$ , the equation becomes:

423

$$\frac{dE_{kin,d}}{dt} = \frac{2}{3} \left( \frac{\rho_g \pi D_0^2 U_0^3}{16 \sqrt{\varepsilon}} \right) \left( f_{kin} \dot{y} \ddot{y} + \frac{1}{2} \frac{df_{kin}}{dy} (\dot{y})^3 \right) \quad (8)$$

424

425 Next, the rate of surface energy is given in eq. (9):

426

$$\frac{dE_{surf,d}}{dt} = \frac{d}{dt} (\sigma S) = \sigma \frac{dS}{dy} \frac{dy}{dt} = \sigma \pi D_0^2 \frac{dS^*}{dy} \frac{dy}{dt} \quad (9)$$

427

428 where  $S^*$  represents the dimensionless droplet surface ( $S^* = S/\pi D_0^2$ ).

429 Introducing the non-dimensional time ( $t^*$ ) the equation becomes:

430

$$\frac{dE_{surf,d}}{dt} = \sigma \pi D_0^2 \frac{dS^*}{dy} \frac{dy}{dt^* \frac{D_0 \sqrt{\varepsilon}}{U_0}} = \frac{\sigma \pi D_0 U_0}{\sqrt{\varepsilon}} \frac{dS^*}{dy} \dot{y} = \left( \frac{\rho_g \pi D_0^2 U_0^3}{16 \sqrt{\varepsilon}} \right) \frac{16}{We} \frac{dS^*}{dy} \dot{y} \quad (10)$$

431

432 In eq. (9), the term  $dS^*/dy$  is a characteristic of the droplet shape and depends on the breakup mode  
 433 and breakup phase (e.g. flattening phase, bag creation, etc). The majority of the breakup models  
 434 assumed ellipsoid shape (either planar or axisymmetric, see Table 2) and provided the term  $dS^*/dy$  as  
 435 a function of the instantaneous deformation  $y$ , using either a simplified analytic formula or a

436 polynomial fitting. Although the assumption of an ellipsoidal shape is an oversimplification it reflects  
 437 with low error the droplet surface area when compared with the results of CFD (comparison not  
 438 presented here).

439 For the pressure work term, it is assumed that this is obtained by multiplying a reference force ( $F_{ref}$ )  
 440 with the reference deformation velocity  $U_{def,y}$ :

441

$$\dot{W}_g = f_{press} \cdot F_{ref} \cdot U_{def,y} = f_{press} \frac{1}{2} \rho_g u_{rel}^2 \frac{\pi D_0^2}{4} \frac{dR}{dt} \quad (11)$$

442

443 The introduction of non-dimensional numbers:  $y$ ,  $t^*$  and  $u_{rel}^* = \frac{u_{rel}}{U_0}$ , gives:

444

$$\dot{W}_g = f_{press} \left( \frac{\rho_g U_0^3 \pi D_0^2}{16\sqrt{\varepsilon}} \right) u_{rel}^{*2} \dot{y} \quad (12)$$

445

446 The coefficient  $f_{press}$  is used to account for the effect of pressure distribution around the droplet as also  
 447 the change of frontal area during droplet deformation. In the NLTAB model this term is proportional  
 448 to  $\dot{y}/y$ , while in the model of Rimbert et al. is proportional to  $K_p(y) \cdot \dot{y}$ , where  $K_p$  is a polynomial  
 449 function of  $y$  (see Table 7). The term  $u_{rel}^*$  includes the effect of change of the relative drop-gas velocity;  
 450 the inclusion of this effect implies that an additional equation has to be solved for the droplet motion  
 451 (see [16]), while ignoring this effect, implies that  $u_{rel}^*$  is unity; in the present work, this term has been  
 452 neglected. The CFD simulations showed that  $u_{rel}^* \geq 0.8$  for all examined cases even at the instance of  
 453 breakup, therefore justifying this choice.

454 Finally, for the viscous dissipation term the approximation of NLTAB [37] is used:

455

$$\dot{W}_{vis,d} = f_{vis} 12\mu_L \left( \frac{\partial u_{cm}}{\partial n} \right)^2 \frac{\pi D_0^3}{6} = f_{vis} 2\mu_L \left( \frac{1}{y} \frac{dy}{dt} \right)^2 \pi D_0^3 \quad (13)$$

456

457 With the introduction of the non-dimensional time ( $t^*$ ) and the numbers  $We$  and  $Oh$ , the equation  
 458 becomes:

459

$$\dot{W}_{vis,d} = f_{vis} \left( \frac{\rho_g \pi D_0^2 U_0^3}{16\sqrt{\varepsilon}} \right) 32 \frac{Oh}{\sqrt{We}} \left( \frac{\dot{y}}{y} \right)^2 \quad (14)$$

460

461 The coefficient  $f_{vis}$  is used to account for the effect of energy dissipation in the streamwise direction.  
 462 By substituting equations (8), (10), (12) and (14) into (5), the final expression for  $y$  is derived in (15).  
 463 One more coefficient has been added to the equation for the effect of surface energy ( $f_{st}$ ) and all  
 464 constants have been incorporated inside the parameters.

465

$$\left( f_{kin} \dot{y} + \frac{1}{2} \frac{df_{kin}}{dy} \dot{y}^2 \right) + f_{vis} \frac{Oh}{\sqrt{We}} \frac{\dot{y}}{y^2} + \frac{f_{st}}{We} \frac{dS^*}{dy} = f_{press} u_{rel}^{*2} \quad (15)$$

466

467 By giving the appropriate values to the parameters  $f_{kin}$ ,  $f_{vis}$ ,  $f_{st}$ ,  $f_{press}$  and  $dS^*/dy$ , equation (15)  
 468 matches the equations of the models TAB, NLTAB, DDB and NS, as shown in Table 7. Finally, the values  
 469 of the coefficients can be estimated based on the results of the CFD simulations resulting in a  
 470 completely new model. However, their derivation is complex and is still a work in progress.

471

472

Table 7. Parameters of the unified secondary breakup model to match the various models of the literature.

	TAB	NLTAB	DDB	Bag-NS	M-NS
$f_{kin}$	1	$\frac{\pi^2 + \frac{16}{y^6}}{\pi^2 + 16}$	1	1	1
$f_{vis}$	$4y^2 C_d, C_d=5$	40	$9\pi^2$	16	16
$f_{st}$	$8C_k, C_k=8$	29	$\frac{27\pi^2}{2}$	24	24
$f_{press}$	$4C_f, C_f=1/3$	$\frac{2C_2}{y},$ $C_2=2/3$	$9\pi/8$	$\frac{a^2}{4}y,$ $a = 2\sqrt{2}$	$\frac{a^2}{4}y^n,$ $a = f(We)$
$\frac{dS^*}{dy}$	$y - 1$	Ellipsoid	$(1 - 2y^{-6})y$	$y$	$y$

473

#### 474 **Appendix C. Derivation of the bag-NS model.**

475

Initially, the viscous Navier-Stokes equations in cylindrical axisymmetric coordinates are employed:

476

$$\rho_L \left( \frac{\partial u_r}{\partial t} + u_r \frac{\partial u_r}{\partial r} \right) = -\frac{\partial p}{\partial r} + \mu_L \left[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial u_r}{\partial r} \right) - \frac{u_r}{r^2} \right] \quad (16)$$

477

$$r \frac{\partial h}{\partial t} + \frac{\partial (ru_r h)}{\partial r} = 0 \quad (17)$$

478

479 Moreover, the mass conservation gives:

480

$$h(t) = \frac{D_0^3}{6R^2} \quad (18)$$

481

482 The parameter  $u_r$  is found by substituting eq. (18) into (17) and solving for it:

483

$$u_r = \frac{r}{R} \frac{dR}{dt} \quad (19)$$

484

485 Eq. (16) requires the calculation of the pressure gradient ( $dp/dr$ ). First, the normal stress balance across  
 486 the interface is employed:

487

$$\sigma\kappa = T_{rr}(g) - T_{rr}(l) \quad (20)$$

488

489  $T_{rr} (l)$  and  $T_{rr} (g)$  represent the normal stress components associated with the liquid and the  
 490 surrounding gas, given by  $-p_L(r) + 2\mu_L \frac{\partial u_r}{\partial r}$  and  $-p_g(r)$ , respectively. At  $r=R$  equation (20) gives:

491

$$p_L(R) = p_g(R) + \sigma\kappa + 2\mu_L \frac{\partial u_r}{\partial r} \quad (21)$$

492

493 The gas pressure field around the droplet ( $p_g$ ) can be estimated using the momentum and mass  
 494 conservation in the gas phase, with the assumptions of inviscid flow, incompressible fluid and quasi-  
 495 steady state. Moreover, the local gas flow is assumed to have the structure of a stagnation point:  $U_x =$   
 496  $-aU_\infty/D_0$ ,  $x$  is the coordinate in the streamwise direction and  $a$  is an indicator of the rate of stretching.  
 497 The resulting equation is (22):

498

$$p_g(r, x) = p_g(0) - \rho_g \frac{a^2 U_0^2}{8D_0^2} r^2 + \rho_g \frac{a^2 U_0^2}{8D_0^2} x^2 \quad (22)$$

499

500 At  $x=0$  eq. (22) becomes:

501

$$p_g(r) = p_g(0) - \rho_g \frac{a^2 U_0^2}{8D_0^2} r^2 \quad (23)$$

502

503  $p_g(0)$  is the stagnation pressure at  $r = x = 0$  given by  $p_g(0) = \rho_g U_0^2 / 2$ . Substituting eq. (23) and (19) into  
 504 (21) gives:

505

$$p_L(R) = p_g(0) - \rho_g \frac{a^2 U_0^2}{8D_0^2} R^2 + \frac{2\sigma}{h} + 2\mu_L \frac{\partial u_r}{\partial r} \quad (24)$$

506

507 The curvature is given by  $k = \left(\frac{h(t)}{2}\right)^{-1}$  due to the rounded periphery of the liquid disk. The pressure  
 508 gradient can finally be calculated using eqs. (24) and (18) as:

509

$$\frac{\partial p}{\partial r} \approx \frac{p_L(R) - p_g(R)}{R} = \frac{1}{R} \left( -\rho_g \frac{a^2 U_0^2}{8D_0^2} R^2 + \frac{12\sigma}{D_0^3} R^2 + \frac{2\mu_L}{R} \frac{dR}{dt} \right) \quad (25)$$

510

511 Substituting eqs. (25) and (19) into (16):

512

$$\rho_L \frac{r}{R} \frac{d^2 R}{dt^2} = -\frac{1}{R} \left( -\rho_g \frac{a^2 U_0^2}{8D_0^2} R^2 + \frac{12\sigma}{D_0^3} R^2 + \frac{2\mu_L}{R} \frac{dR}{dt} \right) \quad (26)$$

513

514 The integration from  $r=0$  to  $r=R$  gives:

515

$$\frac{d^2 R}{dt^2} = \left( \rho_g \frac{a^2 U_0^2}{\rho_L 4 D_0^2} - \frac{24 \sigma}{\rho_L D_0^3} - \frac{4 \mu_L}{\rho_L R^3} \frac{dR}{dt} \right) R \quad (27)$$

516

517 Finally, the non-dimensional parameters are introduced:  $We$ ,  $Oh$ ,  $y = R/(D_0/2)$ ,  $t^* = t/t_{sh} \Rightarrow t =$

518  $t^* \frac{D_0 \sqrt{\varepsilon}}{U_0}$ , and the final differential equation for the droplet deformation is given in (28):

519

$$\ddot{y} + 16 \frac{Oh_l}{\sqrt{We_g}} \frac{\dot{y}}{y^2} + \frac{24}{We_g} y = \frac{a^2}{4} y \quad (28)$$

520

## 521 References

- 522 [1] Ashgriz, N., 2011, Handbook of atomization and sprays: theory and applications, Springer Science & Business  
523 Media.
- 524 [2] "ANSYS®FLUENT Theory Guide, 2014, Release 16.0."
- 525 [3] Temkin, S., and Ecker, G. Z., 1989, "Droplet pair interactions in a shock-wave flow field," Journal of Fluid  
526 Mechanics, 202, pp. 467-497.
- 527 [4] Pilch, M., and Erdman, C. A., 1987, "Use of breakup time data and velocity history data to predict the maximum  
528 size of stable fragments for acceleration-induced breakup of a liquid drop," International Journal of Multiphase Flow,  
529 13(6), pp. 741-757.
- 530 [5] Hsiang, L. P., and Faeth, G. M., 1995, "Drop deformation and breakup due to shock wave and steady  
531 disturbances," International Journal of Multiphase Flow, 21(4), pp. 545-560.
- 532 [6] Warnica, W. D., Rensizbulut, M., and Strong, A. B., 1995, "Drag coefficients of spherical liquid droplets Part 1:  
533 Quiescent gaseous fields," Experiments in Fluids, 18(4), pp. 258-264.
- 534 [7] Feng, Z.-G., and Michaelides, E. E., 2001, "Drag coefficients of viscous spheres at intermediate and high  
535 Reynolds numbers," Journal of Fluids Engineering, 123(4), pp. 841-849.
- 536 [8] Quan, S., and Schmidt, D. P., 2006, "Direct numerical study of a liquid droplet impulsively accelerated by  
537 gaseous flow," Physics of Fluids (1994-present), 18(10), p. 102103.
- 538 [9] Wadhwa, A. R., Magi, V., and Abraham, J., 2007, "Transient deformation and drag of decelerating drops in  
539 axisymmetric flows," Physics of Fluids (1994-present), 19(11), p. 113301.
- 540 [10] Khare P., V. Y., "Drag Coefficients of Deforming and Fragmenting Liquid Droplets," Proc. ILASS Americas,  
541 25th Annual Conference on Liquid Atomization and Spray Systems.
- 542 [11] Kékesi, T., Amberg, G., and Prah Wittberg, L., 2014, "Drop deformation and breakup," International Journal of  
543 Multiphase Flow, 66, pp. 1-10.
- 544 [12] Jain, M., Prakash, R. S., Tomar, G., and Ravikrishna, R. V., 2015, "Secondary breakup of a drop at moderate  
545 Weber numbers," Proceedings of the Royal Society A: Mathematical, Physical and Engineering Science, 471(2177).
- 546 [13] Strotos, G., Malgarinos, I., Nikolopoulos, N., and Gavaises, M., 2016, "Numerical investigation of aerodynamic  
547 droplet breakup in a high temperature gas environment," Fuel, 181, pp. 450-462.
- 548 [14] Yang, W., Jia, M., Sun, K., and Wang, T., 2016, "Influence of density ratio on the secondary atomization of  
549 liquid droplets under highly unstable conditions," Fuel, 174, pp. 25-35.
- 550 [15] Shao, C., Luo, K., and Fan, J., 2017, "Detailed numerical simulation of unsteady drag coefficient of deformable  
551 droplet," Chemical Engineering Journal, 308, pp. 619-631.
- 552 [16] Stefanitsis, D., Malgarinos, I., Strotos, G., Nikolopoulos, N., Kakaras, E., and Gavaises, M., 2017, "Numerical  
553 investigation of the aerodynamic breakup of Diesel and heavy fuel oil droplets," International Journal of Heat and  
554 Fluid Flow, 68, pp. 203-215.
- 555 [17] Stefanitsis, D., Malgarinos, I., Strotos, G., Nikolopoulos, N., Kakaras, E., and Gavaises, M., 2018, "Numerical  
556 investigation of the aerodynamic breakup of droplets in tandem," International Journal of Multiphase Flow.
- 557 [18] Chou, W. H., and Faeth, G. M., 1998, "Temporal properties of secondary drop breakup in the bag breakup  
558 regime," International Journal of Multiphase Flow, 24(6), pp. 889-912.
- 559 [19] Kulkarni, V., and Sojka, P., 2014, "Bag breakup of low viscosity drops in the presence of a continuous air jet,"  
560 Physics of Fluids, 26(7), p. 072103.
- 561 [20] Hsiang, L. P., and Faeth, G. M., 1992, "Near-limit drop deformation and secondary breakup," International  
562 Journal of Multiphase Flow, 18(5), pp. 635-652.
- 563 [21] Dai, Z., and Faeth, G. M., 2001, "Temporal properties of secondary drop breakup in the multimode breakup  
564 regime," International Journal of Multiphase Flow, 27(2), pp. 217-236.
- 565 [22] Krzeczowski, S. A., 1980, "Measurement of liquid droplet disintegration mechanisms," International Journal  
566 of Multiphase Flow, 6(3), pp. 227-239.
- 567 [23] Cao, X.-K., Sun, Z.-G., Li, W.-F., Liu, H.-F., and Yu, Z.-H., 2007, "A new breakup regime of liquid drops identified  
568 in a continuous and uniform air jet flow," Physics of Fluids, 19(5), p. 057103.

569 [24] Gel'Fand, B., Gubin, S., and Kogarko, S., 1974, "Various forms of drop fractionation in shock waves and their  
570 special characteristics," *Journal of Engineering Physics and Thermophysics*, 27(1), pp. 877-882.

571 [25] Zhao, H., Liu, H.-F., Xu, J.-L., Li, W.-F., and Lin, K.-F., 2013, "Temporal properties of secondary drop breakup  
572 in the bag-stamen breakup regime," *Physics of Fluids*, 25(5), p. 054102.

573 [26] O'Rourke, P. J., Amsden, A. A., and Society of Automotive, E., 1987, *The tab method for numerical calculation  
574 of spray droplet breakup*, Society of Automotive Engineers, Warrendale, PA.

575 [27] Lee, M. W., Park, J. J., Farid, M. M., and Yoon, S. S., 2012, "Comparison and correction of the drop breakup  
576 models for stochastic dilute spray flow," *Applied Mathematical Modelling*, 36(9), pp. 4512-4520.

577 [28] Kim, S., Hwang, J. W., and Lee, C. S., 2010, "Experiments and modeling on droplet motion and atomization of  
578 diesel and bio-diesel fuels in a cross-flowed air stream," *International Journal of Heat and Fluid Flow*, 31(4), pp.  
579 667-679.

580 [29] Marek, M., 2013, "The double-mass model of drop deformation and secondary breakup," *Applied Mathematical  
581 Modelling*, 37(16-17), pp. 7919-7939.

582 [30] Villermaux, E., and Bossa, B., 2009, "Single-drop fragmentation determines size distribution of raindrops,"  
583 *Nature Physics*, 5, p. 697.

584 [31] Opfer L., I. V. R., C. Tropea, 2012, "Aerodynamic Fragmentation of Drops: Dynamics of the Liquid Bag,"  
585 ICLASS 2012, 12th Triennial International Conference on Liquid Atomization and Spray Systems Heidelberg,  
586 Germany.

587 [32] Detkovskii, D., and Frolov, S., 1994, "Model of the deformation of a liquid droplet in a gas flow," *Journal of  
588 applied mechanics and technical physics*, 35(6), pp. 911-919.

589 [33] Wang, C., Chang, S., Wu, H., and Xu, J., 2014, "Modeling of drop breakup in the bag breakup regime," *Applied  
590 Physics Letters*, 104(15), p. 154107.

591 [34] Wang, C., Chang, S., Wu, H., Ding, L., and Thompson, J., 2015, "Theoretical Modeling of Spray Drop  
592 Deformation and Breakup in the Multimode Breakup Regime," *Atomization and Sprays*, 25(10).

593 [35] Ibrahim, E., Yang, H., and Przekwas, A., 1993, "Modeling of spray droplets deformation and breakup," *Journal  
594 of Propulsion and Power*, 9(4), pp. 651-654.

595 [36] Rimbart, N., Hajjar, A., Castrillon-Escobar, S., Meignen, R., and Gradeck, M., 2014, "A New Look at the Droplet  
596 Deformation and Breakup Model," *ILASS*.

597 [37] Schmehl, R., 2002, "Advanced modeling of droplet deformation and breakup for CFD analysis of mixture  
598 preparation," *Zaragoza*, 9(11).

599 [38] Bartz, F., Schmehl, R., Koch, R., and Bauer, H., "An extension of dynamic droplet deformation models to  
600 secondary atomization," *Proc. 23rd Annual Conference on Liquid Atomization and Spray Systems, Brno*.

601 [39] Bartz, F., Guildenbecher, D., Schmehl, R., Koch, R., Bauer, H., and Sojka, P., "Model comparison for single  
602 droplet fragmentation under varying accelerations," *Proc. 24th European conference on liquid atomization and  
603 spray systems*.

604 [40] Sichani, A. B., and Emami, M. D., 2015, "A droplet deformation and breakup model based on virtual work  
605 principle," *Physics of Fluids*, 27(3), p. 032103.

606 [41] Wierzbna, A., and Takayama, K., 1988, "Experimental investigation of the aerodynamic breakup of liquid drops,"  
607 *AIAA Journal*, 26(11), pp. 1329-1335.

608 [42] Majithia, A., Hall, S., Harper, L., and Bowen, P., "Droplet breakup quantification and processes in constant and  
609 pulsed air flows," *Proc. Proceedings of the 22nd Conference on Liquid Atomization and Spray Systems (ILASS-  
610 Europe)*, Como Lake, Italy.

611 [43] O'Rourke, P. J., and Amsden, A. A., 1987, "The TAB method for numerical calculation of spray droplet breakup,"  
612 No. 0148-7191, SAE Technical Paper.

613 [44] Hirt, C. W., and Nichols, B. D., 1981, "Volume of fluid (VOF) method for the dynamics of free boundaries,"  
614 *Journal of Computational Physics*, 39(1), pp. 201-225.

615 [45] Lafaurie, B., Nardone, C., Scardovelli, R., Zaleski, S., and Zanetti, G., 1994, "Modelling Merging and  
616 Fragmentation in Multiphase Flows with SURFER," *Journal of Computational Physics*, 113(1), pp. 134-147.

617 [46] "ANSYS@FLUENT, 2014, Release 16.0."

618 [47] Jain, S. S., Tyagi, N., Prakash, R. S., Ravikrishna, R., and Tomar, G., 2018, "Secondary breakup of drops at  
619 moderate Weber numbers: Effect of Density ratio and Reynolds number," *arXiv preprint arXiv:1803.02989*.

620 [48] Liang, C., 2016, "Computational methods for the investigation of liquid drop phenomena in external gas flows."

621 [49] Malgarinos, I., Nikolopoulos, N., and Gavaises, M., 2015, "Coupling a local adaptive grid refinement technique  
622 with an interface sharpening scheme for the simulation of two-phase flow and free-surface flows using VOF  
623 methodology," *Journal of Computational Physics*, 300, pp. 732-753.

624 [50] G. Strotos, I. M., N. Nikolopoulos, K. Papadopoulos, A. Theodorakakos, M. Gavaises, 2015, "Performance of  
625 VOF methodology in predicting the deformation and breakup of impulsively accelerated droplets," *ICLASS 2015,  
626 13th Triennial International Conference on Liquid Atomization and Spray Systems, August 23-27 Tainan, Taiwan*.

627 [51] Strotos, G., Malgarinos, I., Nikolopoulos, N., and Gavaises, M., 2016, "Predicting droplet deformation and  
628 breakup for moderate Weber numbers," *International Journal of Multiphase Flow*, 85, pp. 96-109.

629 [52] Strotos, G., Malgarinos, I., Nikolopoulos, N., and Gavaises, M., 2016, "Aerodynamic breakup of an n-decane  
630 droplet in a high temperature gas environment," *Fuel*, 185, pp. 370-380.

631 [53] Stefanitsis, D., Malgarinos, I., Strotos, G., Nikolopoulos, N., Kakaras, E., and Gavaises, M., 2017, "Numerical  
632 investigation of the aerodynamic breakup of Diesel droplets under various gas pressures," 28th Conference on  
633 Liquid Atomization and Spray Systems (ILASS-Europe 2017)Valencia, Spain.

634 [54] Malgarinos, I., Nikolopoulos, N., Marengo, M., Antonini, C., and Gavaises, M., 2014, "VOF simulations of the  
635 contact angle dynamics during the drop spreading: Standard models and a new wetting force model," *Advances in  
636 Colloid and Interface Science*, 212, pp. 1-20.

637 [55] Malgarinos, I., Nikolopoulos, N., and Gavaises, M., 2016, "A numerical study on droplet-particle collision  
638 dynamics," *International Journal of Heat and Fluid Flow*, 61, Part B, pp. 499-509.

639 [56] Malgarinos, I., Nikolopoulos, N., and Gavaises, M., 2017, "Numerical investigation of heavy fuel droplet-particle  
640 collisions in the injection zone of a Fluid Catalytic Cracking reactor, Part I: Numerical model and 2D simulations,"  
641 *Fuel Processing Technology*, 156, pp. 317-330.

642 [57] Malgarinos, I., Nikolopoulos, N., and Gavaises, M., 2017, "Numerical investigation of heavy fuel droplet-particle  
643 collisions in the injection zone of a Fluid Catalytic Cracking reactor, part II: 3D simulations," *Fuel Processing  
644 Technology*, 156, pp. 43-53.

645 [58] Strotos, G., Malgarinos, I., Nikolopoulos, N., and Gavaises, M., 2016, "Predicting the evaporation rate of  
646 stationary droplets with the VOF methodology for a wide range of ambient temperature conditions," *International  
647 Journal of Thermal Sciences*, 109, pp. 253-262.

648 [59] Guildenbecher, D. R., López-Rivera, C., and Sojka, P. E., 2009, "Secondary atomization," *Experiments in  
649 Fluids*, 46(3), pp. 371-402.

650 [60] Aalburg, C., 2002, Deformation and breakup of round drops and nonturbulent liquid jets in uniform crossflows.

651 [61] Liu, Z., and Reitz, R. D., 1997, "An analysis of the distortion and breakup mechanisms of high speed liquid  
652 drops," *International Journal of Multiphase Flow*, 23(4), pp. 631-650.

653 [62] Nicholls, J. A., and Ranger, A. A., 1969, "Aerodynamic shattering of liquid drops," *AIAA Journal*, 7(2), pp. 285-  
654 290.

655 [63] Schlotke, M., 2011, "Analytical Investigation of Droplet Breakup in Accelerated Flow," PhD thesis, Universität  
656 Stuttgart.

657 [64] Dormand, J. R., and Prince, P. J., 1980, "A family of embedded Runge-Kutta formulae," *Journal of  
658 computational and applied mathematics*, 6(1), pp. 19-26.

659 [65] Shampine, L. F., and Reichelt, M. W., 1997, "The matlab ode suite," *SIAM journal on scientific computing*,  
660 18(1), pp. 1-22.

661

662