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Improved droplet breakup models for spray applications

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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 examined. 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]

ε Density ratio [-]

μ Dynamic viscosity [kg/(m·s)]

ρ Density [kg/m³]

σ Surface tension [N/m]

Subscripts/Superscripts

* Non-dimensional quantity

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

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 (Figure 2) and several models have been developed for its
46 estimation as a function of time. These can be classified into empirical correlations based on
47 experimental observations and semi-analytic/theoretical models, which are based on physical
48 principles.

49 Various studies in the literature conducted experiments of aerodynamic droplet breakup and based
50 on their results they proposed empirical correlations for the prediction of the droplet deformation as
51 a function of the non-dimensional time. These correlations can be written in the general form of $y=$

52 $c_0+c_1(t^*)^{c_2}+c_3(t^*)^2$, where y is the non-dimensional deformation (Figure 2), whilst the coefficients $c_0, c_1,$
53 c_2 and c_3 are summarized for each study in Table 1, along with their range and conditions of
54 applicability. Apparently, these correlations perform quite well when compared against the
55 experimental data that they were based upon, and the question arises is if they also perform well
56 against other data at a) similar conditions and b) at different breakup modes. This is addressed in
57 Appendix A in which the model results are compared against the experimental data of [12, 18-22] in
58 the three main breakup regimes (bag, multi-mode and sheet-thinning) for Weber numbers in the range
59 of 15 to 101. In the bag breakup regime ($We=15-20$) the model of Chou and Faeth [18] shows the best
60 agreement with the experimental data, in the multi-mode regime ($We=52.6$) that of Cao et al. [23] and
61 in the sheet-thinning regime the model of Gel'fand et al. [24] ($We=101$). None of the models is able to
62 accurately predict the droplet deformation in all the examined regimes.

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

Study	General equation: $y=c_0+c_1(t^*)^{c_2}+c_3(t^*)^2$				Conditions of applicability ^{*1}		
	c_0	c_1	c_2	c_3	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	$t^* \leq 1.5$

65
66 ¹Refers to the conditions of the experiments that the corresponding model was based upon. The models are
67 generally valid for low Oh numbers

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

76 that the TAB model shows good agreement with the experiment of Krzeczowski [22] for the breakup
77 of a water droplet with $We=101$. Later, Kim et al. [28] tuned these coefficients to match the results of
78 their experiments for Diesel droplets at We numbers in the range of 9.6 up to 26.6. Finally, Marek [29]
79 introduced another degree of freedom to the mathematical formulation of TAB, so as to include also
80 the translational motion of the droplet. A second mass was added to the system, which could move
81 and oscillate independently, and thus the system resembled the system configuration of a double
82 mass-spring-damper giving the name to the model as double mass TAB (DMTAB). The DMTAB is
83 applicable to the deformation and bag breakup regimes and its advantage over the TAB model is that
84 it can treat cases with low density ratios (ϵ) and high Oh numbers, in which the droplet translational
85 velocity changes significantly.

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

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

98 Regarding the theoretical models based on the conservation of energy, Ibrahim et al. [35] developed
99 the so called deformation and breakup model (DDB), which is applicable to deforming droplets for We
100 numbers greater than 20. Rimbart et al. [36] improved the DDB model by assuming potential flow
101 around the droplet and extensional flow (i.e. with no shear) inside the droplet. The resulting model
102 showed acceptable agreement with the experimental data of [22, 31] for We numbers equal to 11.5,
103 18.4 and 103.5, while the agreement was not good for the case of $We=13.5$. Schmehl and co-workers
104 [37, 38] utilized the mechanical energy balance on the droplet to derive a non-linear differential
105 equation similar to that of TAB, which they named non-linear TAB (NLTAB). This equation accounts for
106 the modification of the aerodynamic forces imposed by the deformation of the droplet, and it showed
107 good agreement with the experimental data of [21, 39] for the time variation of droplet deformation.
108 Finally, Sichani and Emami [40] utilized the virtual work principle to describe the droplet deformation
109 in the deformation and bag breakup regimes. The results of the model showed good agreement with
110 the experimental data of [18, 21, 22, 41, 42] for We numbers ranging from 12.5 up to 20.

111 The aforementioned theoretical models are summarized in Table 2 along with their basic
112 characteristics. In addition, the performance of selected models (TAB, DDB, NLTAB, Rimbart et al. [36]
113 and Kulkarni and Sojka [19]) is evaluated by comparing their results with the experimental data of [12,
114 18-22] in the three breakup regimes (bag, multi-mode and sheet-thinning) for $We=15-101$, as
115 presented in Appendix A. For $We=15$ the model of Kulkarni and Sojka [19] agrees well with the
116 experimental data, while for $We=52.6$ and $We=110$ the DDB model gives the best results overall. For

117 $We=20$ all models deviate from the experimental data. Similar to the empirical models, none of the
 118 examined theoretical models is able to accurately predict the droplet deformation in all the examined
 119 regimes.

120

121

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	$\gamma_{cr}=2$	3	-
NLTAB [37, 38]	Energy balance	Ellipsoid	Spatial	Yes	No	$\gamma_{cr}=1.8$ and $\dot{\gamma}=0$ or $\gamma_{cr}=2.1$	1	-
DMTAB [29]	Momentum conservation	Ellipsoid	Uniform	No	Yes	$\gamma_{cr}=2$	3	$We \leq 50$, large and small ϵ and Oh
DDB [35]	Energy balance	Elliptic cylinder	Uniform	No	No	$\gamma_{cr}=(We/2)/(6\pi)$	0	$We > 20$
Rimbert et al. [36]	Energy balance	Ellipsoid	Spatial (potential flow)	Yes (homotetical deformation)	Yes	$\gamma_{cr}=2$	0	-
BTB [32-34]	Linear strain equation	Ellipsoid	Uniform	No	No	$(B^{-1}+B^5-2B^4)/30 > We$, $B=(3\pi/4)\gamma$	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 Emami [40]	Lagrange -type equation s of motion	Bag	Spatial	Yes	No	$\frac{4}{3} \frac{1 - K^*2}{y_1^2 + y_2^2}$	1	$We \leq 20,$ $Re > 100,$ $\epsilon > 500,$
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122

123 ¹Applicability is based on the original paper proposing the model.

124 ² K is a parameter; y_1 and y_2 are the deformations in both axes.

125

126 The aforementioned observations lead to the conclusion that there is a lack of a single accurate enough
 127 model for the prediction of droplet deformation for a wide range of We numbers in the three basic
 128 breakup regimes: i) bag, ii) multi-mode and iii) sheet-thinning. So far, the TAB model is widely used in
 129 spray codes due to its simplicity, since it has an analytic solution. However, it predicts purely oscillatory
 130 deformation for all breakup regimes, something that is not realistic (see Figures 4 to 6). On the other
 131 hand, the recently developed model of Kulkarni and Sojka [19] (termed as bag-Navier-Stokes or bag-NS
 132 for the remaining of the paper) predicts an exponential growth, which agrees well with experimental
 133 observations for the bag breakup mode, but it cannot be used to other breakup modes. The scope of
 134 the present work is to extend these two models. Nevertheless, it should be noted that an oscillatory
 135 deformation superimposed to an exponential function might result in a more accurate model,
 136 however, its implementation is complicated, possibly without significantly improving its performance
 137 compared to the models that follow one of the two approaches.

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

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

152

153 **2 Computational setup and examined conditions**

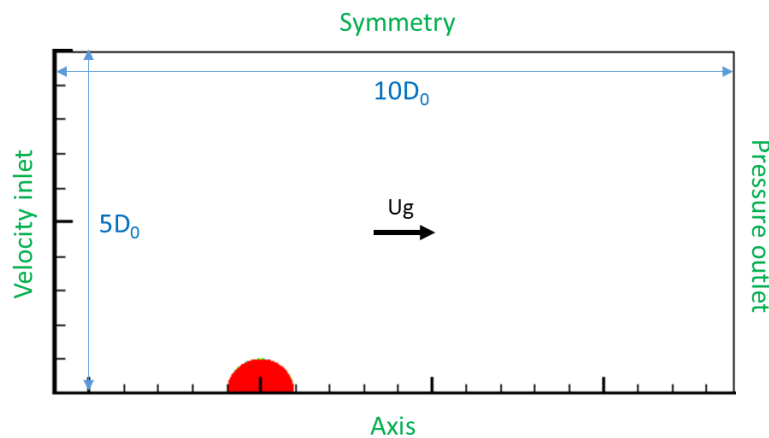
154 Apart from utilizing experimental data for the estimation of the model parameters, complimentary
 155 CFD simulations have also been performed. The CFD simulations are utilized for the derivation of the
 156 parameters of the improved TAB and M-NS models in the multi-mode and sheet-thinning regimes,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

159 deformation, which is necessary for the extraction of a breakup condition that is utilized in both
160 breakup models.

161 The numerical CFD model solves the Navier-Stokes equations coupled with the Volume of Fluid (VOF)
162 methodology [44] for tracking the interface between the liquid droplet and the surrounding gas. The
163 surface tension forces are modelled with the Continuum Surface Stress (CSS) model of [45]. The
164 simulations are performed in a two-dimensional axisymmetric domain with the commercial CFD tool
165 ANSYS FLUENT v16 [46]. At low Reynolds numbers, such as those examined in this work (Table 4), the
166 axisymmetric approximation has proven to be relatively accurate during the deformation stages of
167 breakup [16, 47, 48]. Various User Defined Functions (UDFs) are employed for i) the adaptive local grid
168 refinement technique around the liquid-gas interface [49], ii) the adaptive time-step scheme for the
169 implicit VOF solver based on the velocity at the droplet interface [13], and iii) the moving mesh
170 technique based on the average velocity of the droplet. The CFD model has been developed and
171 validated in previous works for the case of aerodynamic droplet breakup [13, 16, 17, 50-53], as well as
172 for other applications such as the free fall of droplet [49], the droplet impingement on a flat wall [54]
173 or a spherical particle [55-57], and the droplet evaporation [13, 52, 58].

174 The 2-dimensional axisymmetric computational domain and boundary conditions are presented in
175 Figure 1. The droplet is initially stagnant, while air flows from the left boundary with a constant velocity
176 U_g , causing it to move and deform. The computational cells have a rectangular shape with a base grid
177 resolution equal to $3cpR$ (cells per radius), while 6 levels of local grid refinement are applied to obtain
178 the desired resolution of $192cpR$ around the liquid-gas interface. The resolution of $192cpR$ is adequate
179 for the simulations of droplet breakup, since simulations with 48, 96, 192 and 384cpR have shown that
180 the average drop velocity and deformation change less than 1% when a finer grid is used.

181



182

183 Figure 1. Computational domain and boundary conditions for the CFD simulations.

184

185 The liquid properties correspond to those of Diesel fuel, while the surrounding gas is air at temperature
186 of 293.15K and pressure of 1bar (energy equation not solved). Although Diesel is utilized as test fuel in
187 the current work, the results can be considered valid for low viscosity fuels as long as the Ohnesorge
188 number is kept below 0.1 [59]. The same is true for the effect of ambient pressure or equivalently that
189 of the density ratio, which becomes important approximately below 32 [53, 60]. Both the properties
190 of Diesel and air as well as the droplet diameter are based on [61] as presented in Table 3. The

191 corresponding non-dimensional numbers are $\epsilon=678$, $Oh=0.038$ and $N=117$ (eq. (3)). The high density
 192 ratio (ϵ) and low Oh number ensure that their effect is minimized, focusing only on the effect of We
 193 number. By altering the gas velocity, the resulting We numbers range from 20 up to 350, resulting in
 194 21 simulations in the three breakup regimes, i.e. those of bag, multi-mode and sheet-thinning, as
 195 shown in Table 4. The corresponding Re numbers range from 531 to 2221.

196
 197 Table 3. Properties of liquid Diesel and air at $T=293.15K$ and $P=1bar$ based on [61].

D_0 (μm)	P (bar)	T_g (K)	μ_g (kg/s·m)	ρ_g (kg/m ³)	T_L (K)	μ_L (kg/m·s)	ρ_L (kg/m ³)	σ (N/m)
198	1	293.15	1.85E-05	1.215	293.15	0.00217	824	0.02

198
 199 Table 4. Examined cases of CFD simulations.

Case	$U_{g,o}$ (m/s)	We	Re	Oh	ϵ	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

200
 201 **3 Mathematical model**

202 **3.1 Non-dimensional numbers**

203 The non-dimensional numbers that are commonly used to describe the breakup of isolated droplets
 204 are the Weber (We), Ohnesorge (Oh) and Reynolds (Re) numbers as well as the density (ϵ) and viscosity
 205 ratios (N) of the two phases [59].

206

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

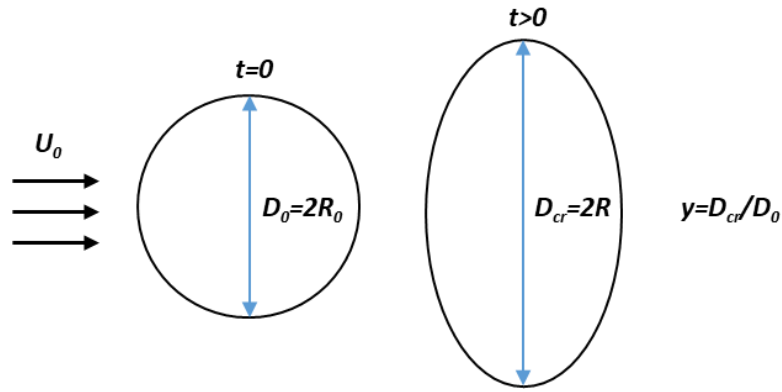
207
208
209
210

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

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

211
212
213
214
215

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.



216
217
218

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:

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

224

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

235

236 parameter C_d is taken constant and equal to 10, in agreement with [29, 63]; this parameter is expected
 237 to be a function of Oh number, which has a constant low value throughout this study and has a minor
 238 effect on the breakup process.

239
 240

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						$0, We \geq 60$

241

242 3.3 Modified Navier-Stokes (M-NS) model

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

251 In the M-NS model the droplet deformation is described by equation (4). The difference with the
 252 original bag-NS model lies in the estimation of the pressure term, which is a function of y^n instead of y
 253 (4th term from the left of eq. (4)). Eq. (4) is a second-order non-linear differential equation with no
 254 analytical solution, the numerical solution of which is obtained in this work using an explicit 4th order
 255 Runge-Kutta method [64, 65].

256

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

257

258 The parameter a is called rate of stretching, while the parameter n is called pressure exponent and has
 259 been introduced in the present work to provide a more flexible numerical consideration of the
 260 pressure contribution. For $n \geq 1$ the deformation grows exponentially in time (note that $n=1$
 261 corresponds to the original model of [19], as shown in Table 6), while for $n < 1$ the deformation becomes
 262 oscillatory. More specifically, for $n=0$ the equation becomes similar to that of the TAB model, while for
 263 $n=-1$ it becomes similar to that of the NLTAB, since the pressure term is proportional to $1/y$. For each
 264 breakup mode, the value of n that gives the higher coefficient of determination (R^2) is selected,
 265 compared to the results of the experimental studies of [12, 18-21] (bag regime) and the CFD
 266 simulations (multi-mode and sheet-thinning regimes), as shown in Table 6.

267 Finally, instead of using a constant value for the parameter a , the current study proposes this to be a
 268 function of the We number for each breakup mode (bag, multi-mode and sheet-thinning), as presented
 269 in Table 6. For the bag breakup regime, the experimental data of [12, 18-21] for the temporal evolution

270 of droplet deformation are utilized, while for the multi-mode and sheet-thinning regimes the results
 271 of the CFD simulation are employed instead; α is found for each We number by fitting eq. (4) to the
 272 results and by assuming a linear dependence on the We number. It should be mentioned that the
 273 equation of α in the bag breakup regime gives a value of a equal to 2.88 for $We=15$, which is close to
 274 the value of 2.83 proposed by [19] for the same We (Table 6).

275
 276

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

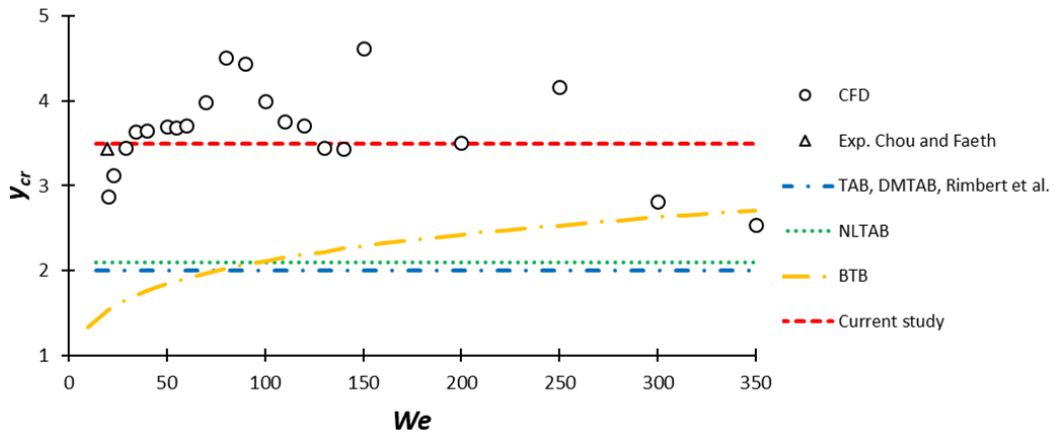
Breakup mode	Original bag-NS		Proposed M-NS	
	n	α	n	α
Bag	1	2.83	1	$3.6 - 0.048We$
Multi-mode	-	-	-0.5	$3.35 + 0.0032We$
Sheet-thinning	-	-	2	$2.35 + 0.0042We$

277

278 3.4 Breakup condition

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

287



288

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

291

292 4 Results and discussion

293 The temporal evolution of droplet deformation can be calculated using the two models (improved TAB
 294 and M-NS) with their respective equations and parameters: i) improved TAB model using eq. (3) and
 295 the parameters of Table 5 and ii) M-NS model using eq. (4) and the parameters of Table 6. The results

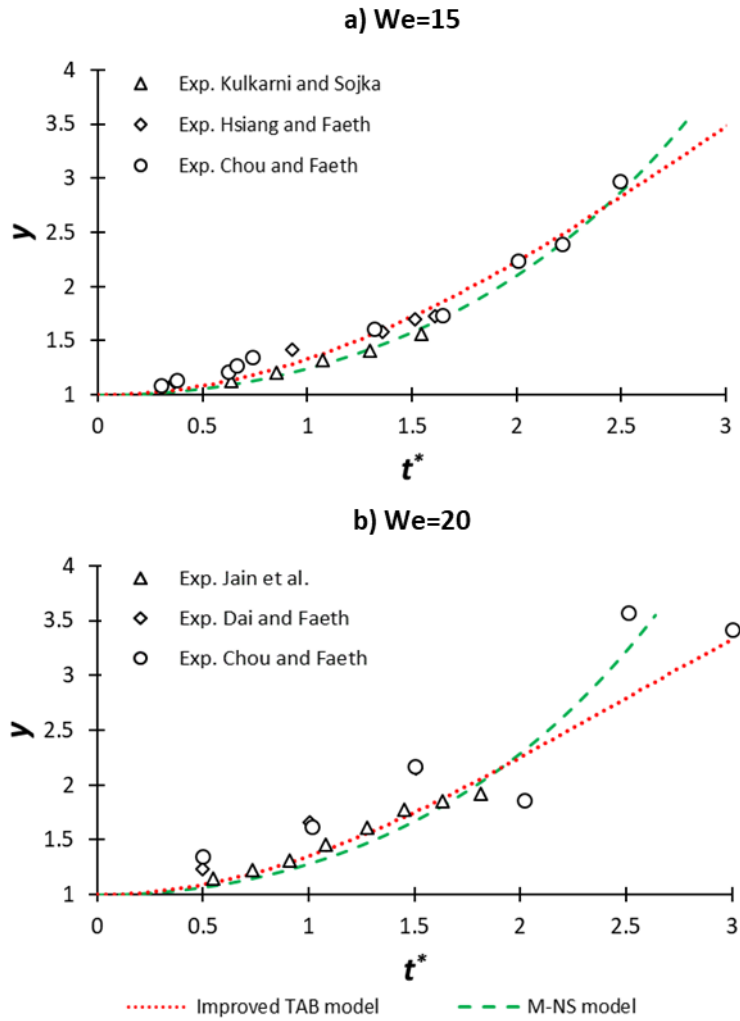
296 are presented in the following sub-sections as calculated by the two models in the bag, multi-mode
297 and sheet-thinning regimes, against the results of experimental studies (bag breakup regime) and
298 those of the CFD simulations (multi-mode and sheet-thinning regimes).

299

300 **4.1 Bag breakup regime - $We=10-20$**

301 The results of two breakup models (improved TAB and M-NS) are illustrated in Figure 4 for two We
302 numbers in the bag breakup regime ($We=15$ and 20), along with those of the experimental studies for
303 the same We numbers [12, 18-21]. Both models show a good agreement with the experimental data
304 for both We numbers. The TAB model predicts lower values for the deformation compared to the M-
305 NS model at higher t^* (≥ 2.5), owing to the assumption that the droplet deformation is modeled as an
306 oscillation in the TAB model, in comparison with the exponential behavior predicted by the M-NS
307 model. It should be noted that the experimental data of Chou and Faeth [18] exhibit a fluctuation for
308 the case of $We=20$ and at $t^*\geq 2$, something that pertains to a combined exponential and oscillatory
309 droplet deformation. This behavior is also observed in the simulations of Figure 5 and Figure 6 and it
310 is something that has not been reported before in the literature. Nevertheless, the exponential part
311 seems to dominate, while further experimental and numerical studies are required to verify this
312 observation.

313



314

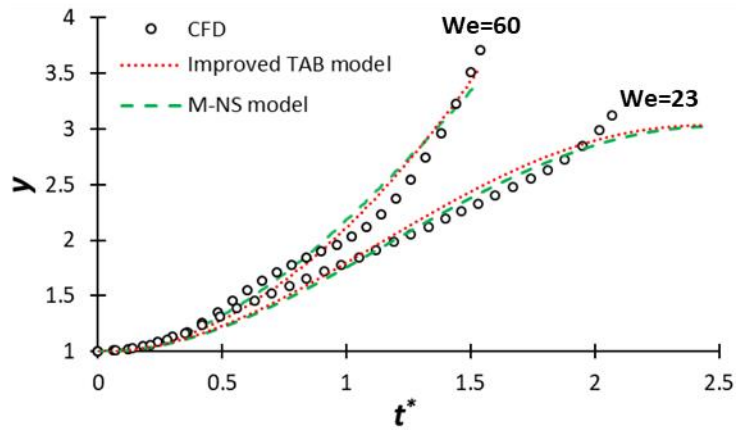
315 Figure 4. Temporal evolution of droplet deformation as predicted by the improved TAB and M-NS models
 316 along with the experimental data from the literature for a) $We=15$ and b) $We=20$.

317

318 **4.2 Multi-mode breakup regime - $We=21-65$**

319 The results of the two breakup models are presented in Figure 5 for two We numbers, 23 and 60, in
 320 the multi-mode regime, along with those of the simulations for the same We numbers. The agreement
 321 is good between the models and the simulations, apart from the prediction of a slightly higher breakup
 322 initiation time for the case of $We=23$. This is attributed to the oscillatory behavior of the models and
 323 the consequent occurrence of breakup at the time when $\dot{\gamma}=0$ and not at $\gamma_{cr}=3.5$. Note that a selection
 324 of an exponential solution for the M-NS model (parameter $n \geq 1$), although it gives slightly better results
 325 for the case of $We=60$, it does not agree will with the simulations for the case of $We=23$, and therefore
 326 is not selected.

327



328

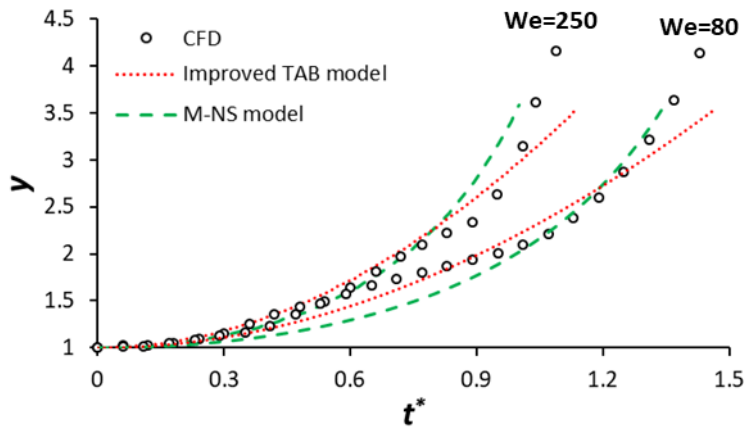
329 Figure 5. Temporal evolution of droplet deformation as predicted by the improved TAB and M-NS models with
 330 the results of the simulations for two We numbers in the multi-mode regime (60 and 23).
 331

331

332 4.3 Sheet-thinning breakup regime - $We=66-350$

333 In Figure 6 the results from the two breakup models are presented for two We numbers (80 and 250)
 334 in the sheet-thinning regime, along with those of the simulations for the same We numbers. Good
 335 agreement is observed again for both models, although a slight underestimation of y_{cr} is noticed for
 336 both We numbers, due to the higher value of y_{cr} as predicted by the simulations in the current regime.
 337 In addition, the results of the M-NS model are closer to those of the simulations due to their steeper
 338 inclination.
 339

339



340

341 Figure 6. Temporal evolution of droplet deformation as predicted by the improved TAB and M-NS models
 342 along with the results of the simulations for two We numbers in the sheet-thinning regime (80 and 250).
 343

343

344 5 Conclusions and future work

345 The present work examined the droplet deformation and breakup models for the three basic regimes
 346 of droplet breakup, i.e. the bag, multi-mode and sheet-thinning. The publicly available empirical
 347 models of [18, 20, 23, 24] were examined as well as the theoretical models TAB, DDB, NLTAB, Rimbert
 348 et al. [36] and bag-NS [19], for their range of validity against available experimental data ($We=15-101$).
 349 It was found (see Appendix A) that none of them was capable of accurately predicting the droplet

350 deformation in all the three breakup regimes. For this reason, two existing models were improved and
351 modified, namely i) an improved TAB model and ii) the M-NS model, which is a modified version of an
352 existing model based on the Navier-Stokes equations.

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

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

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

369

370 **Acknowledgements**

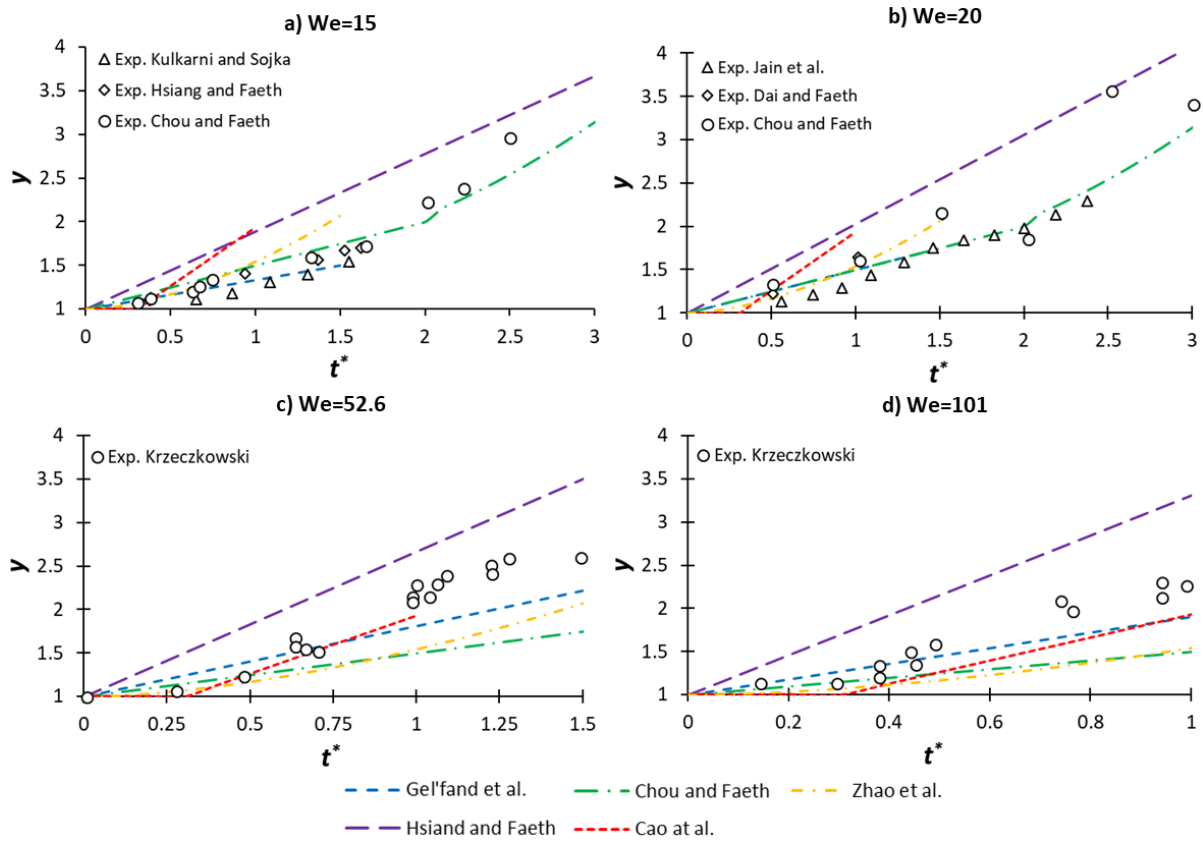
371 Financial support from the MSCA-ITN-ETN of the European Union's H2020 programme, under REA
372 grant agreement n. 675676 is acknowledged.

373

374 **Appendix A. Comparison of the existing deformation and breakup models with** 375 **experimental data.**

376 The temporal evolution of droplet deformation as predicted by the various models of Table 1 and
377 selected models of Table 2 are presented in Figure 7 and Figure 8, respectively, along with various
378 experimental data found in the literature in three breakup regimes (bag, multi-mode and sheet-
379 thinning) for $We=15$ [18-20], $We=20$ [12, 18, 21], $We=52.6$ [22] and $We=101$ [22]. It should be noted
380 that the applicability of some models has been extended beyond the range presented in Table 1 and
381 Table 2 in order to assess if their range of applicability can be extended. The experiments are plotted
382 up to the breakup initiation time, while those by [22] have been shifted in terms of time based on the
383 results of CFD simulations at the same conditions. In the bag breakup regime ($We=15-20$) the empirical
384 model of Chou and Faeth [18] and the theoretical model of Kulkarni and Sojka [19] show the best
385 agreement, in the multi-mode regime ($We=52.6$) that of Cao et al. [23] and the DDB, and in the sheet-
386 thinning regime ($We=101$) that of Gel'fand et al. [24] and the DDB again.

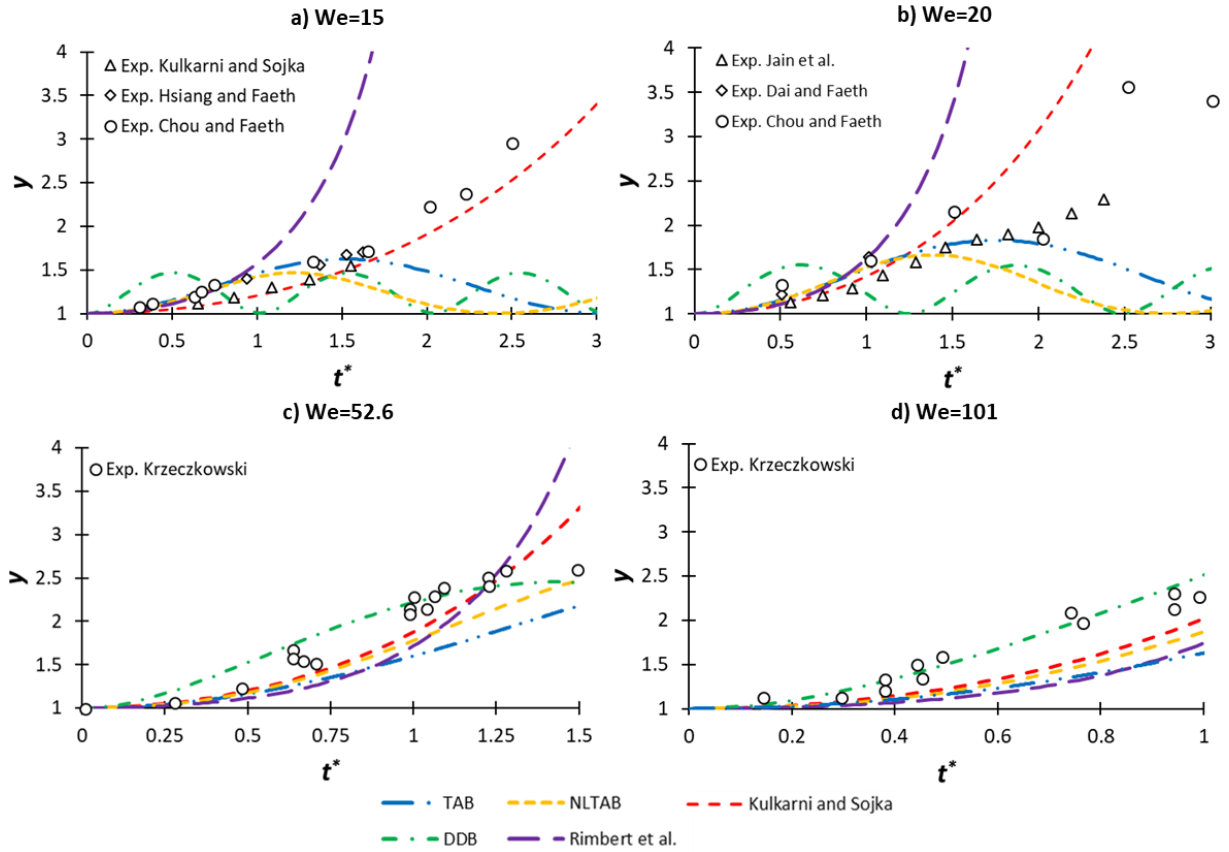
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388

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

391



392

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

395

396 Appendix B. Unified secondary breakup model.

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

406

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

407

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

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

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

415

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

416

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

424 The rate of kinetic energy is:

425

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

426

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

428 $\frac{t}{D_0 \sqrt{\varepsilon}} U_0 \rightarrow t = t^* \frac{D_0 \sqrt{\varepsilon}}{U_0}$, the equation becomes ($\dot{y} = \frac{dy}{dt^*}$):

429

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

430

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

432

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

433

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

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

436

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

437

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

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

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

$$447 \dot{W}_{press} = f_{press} \cdot F_{ref} \cdot U_{def,y} = f_{press} \frac{1}{2} \rho_g u_{rel}^2 \frac{\pi D_0^2}{4} \frac{dR}{dt} \quad (11)$$

448

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

450

$$451 \dot{W}_{press} = f_{press} \left(\frac{\rho_g U_0^3 \pi D_0^2}{16\sqrt{\varepsilon}} \right) u_{rel}^{*2} \dot{y} \quad (12)$$

452

453 The coefficient f_{press} is used to account for the effect of pressure distribution around the droplet as also
 454 the change of frontal area during droplet deformation. In the NLTAB model this term is proportional
 455 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
 456 function of y (see Table 7). The term u_{rel}^* includes the effect of change of the relative drop-gas velocity;
 457 the inclusion of this effect implies that an additional equation has to be solved for the droplet motion
 458 (see [16]), while ignoring this effect, implies that u_{rel}^* is unity. The CFD simulations showed that $u_{rel}^* \geq$
 459 0.8 for all examined cases even at the instance of breakup, where it takes its minimum value.

460 Finally, for the viscous dissipation term the approximation of NLTAB [37] is used (n is the unit vector in
 461 the direction of y):

462

$$463 \dot{W}_{vis,d} = f_{vis} 12\mu_L \left(\frac{\partial u_{cm}}{\partial n} \right)^2 \frac{\pi D_0^3}{6} = f_{vis} 2\mu_L \left(\frac{1}{y} \frac{dy}{dt} \right)^2 \pi D_0^3 \quad (13)$$

464

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

467

$$468 \dot{W}_{vis,d} = f_{vis} \left(\frac{\rho_g \pi D_0^2 U_0^3}{16\sqrt{\varepsilon}} \right) 32 \frac{Oh}{\sqrt{We}} \left(\frac{\dot{y}}{y} \right)^2 \quad (14)$$

469

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

474

$$475 \left(f_{kin} \dot{y} + \frac{1}{2} \frac{df_{kin}}{dy} \dot{y}^2 \right) + f_{vis} \frac{Oh}{\sqrt{We}} \frac{\dot{y}}{y^2} + \frac{f_{st}}{We} \frac{dS^*}{dy} = f_{press} u_{rel}^{*2} \quad (15)$$

476

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

477

478

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
u_{rel}^*	1	1	1	1	1

479

480 Appendix C. Derivation of the bag-NS model.

481 Initially, the viscous Navier-Stokes equations in cylindrical axisymmetric coordinates are employed (see
 482 Figure 9):

483

$$484 \rho_L \left(\frac{\partial u_r}{\partial t} + u_r \frac{\partial u_r}{\partial r} \right) = -\frac{\partial p}{\partial r} + \mu_L \left[\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial u_r}{\partial r} \right) - \frac{u_r}{r^2} \right] \quad (16)$$

484

$$485 r \frac{\partial h}{\partial t} + \frac{\partial(r u_r h)}{\partial r} = 0 \quad (17)$$

485

486 Moreover, the mass conservation gives the rim thickness as:

487

$$488 h(t) = \frac{D_0^3}{6R^2} \quad (18)$$

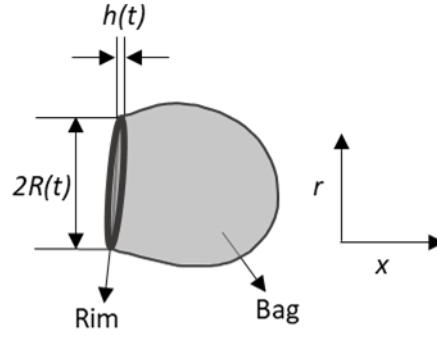


Figure 9. Definition of rim thickness and droplet radius in cylindrical coordinates.

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

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

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

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

$T_{rr}(l)$ and $T_{rr}(g)$ represent the normal stress components associated with the liquid and the 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:

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

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

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

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

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

512 $p_g(0)$ 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
 513 (21) gives:

514

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

515

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

518

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

519

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

521

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

522

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

524

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

525

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

527 $t^* \frac{D_0 \sqrt{\varepsilon}}{U_0}$, and the final differential equation for the droplet deformation is given in (28):

528

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

529

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