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1	Determination of the aerodynamic droplet breakup boundaries based
2	on a total force approach
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23

#### 24 Abstract

25 The determination of the critical  $We_g$  number separating the different breakup regimes 26 has been extensively studied in several experimental and numerical works, while 27 empirical and semi-analytical approaches have been proposed to relate the critical 28  $We_g$  number with the  $Oh_l$  number. Nevertheless, under certain conditions, the  $Re_g$ 29 number and the density ratio  $\varepsilon$  may become important. The present work provides a simple but reliable enough methodology to determine the critical  $We_g$  number as a 30 31 function of the aforementioned parameters in an effort to fill this gap in knowledge. It 32 considers the main forces acting on the droplet (aerodynamic, surface tension and 33 viscous) and provides a general criterion for breakup to occur but also for the 34 transition among the different breakup regimes. In this light, the present work proposes the introduction of a new set of parameters named as  $We_{g,eff}$  and  $Ca_l$ 35 36 monitored in a new breakup plane. This plane provides a direct relation between gas 37 inertia and liquid viscosity forces, while the secondary effects of  $Re_g$  number and density ratio have been embedded inside the effective  $We_g$  number ( $We_{g,eff}$ ) 38

## 39 Keywords: droplet breakup; critical We number; VOF simulations

# 41 **1 Introduction**

The aerodynamic droplet breakup has been extensively studied in experimental and numerical works due to its importance in spray systems. Depending on the relative strength of the main forces acting on the droplet (aerodynamic, surface tension and viscous forces), different breakup types can be observed such as the bag breakup, the transitional breakup (including several sub-types), the sheet-thinning breakup and the catastrophic breakup. A complete description of these breakup modes can be found in the review article of (Guildenbecher et al., 2009) among others.

Increasing the gas phase inertia results in the successive transition between the aforementioned breakup regimes. The parameters affecting droplet breakup are grouped into dimensionless numbers, such as the  $We_g$ , the  $Oh_l$  and the  $Re_g$  numbers, but also the density and viscosity ratios of the liquid/gas phase ( $\varepsilon$  and N respectively); see section 2.1 for a complete description of these numbers. Among them, the  $We_g$ number is the most influential, while the liquid viscous damping becomes important only when  $Oh_l$ >0.1; see for example the breakup map of (Hsiang and Faeth, 1995).

The  $We_g$  number leading to droplet breakup (or generally separating different breakup regimes) is called critical We number ( $We_{g,cr}$ ) and in the limit of negligible liquid viscosity (i.e. low  $Oh_l$ ), we call it in the present work as  $We_{g,cr,0}$  (the subscript 0 denotes negligible viscosity). Having also in mind that the experimental data are characterized by high  $Re_g$  numbers, the  $We_{g,cr,0}$  generally represents negligible viscosity effects both in the gas and liquid phases. In the following paragraphs, the various approaches found in literature to relate  $We_{g,cr,0}$  with  $We_{g,cr,0}$  will be presented. In (Guildenbecher et al., 2009) it is stated that breakup is observed for  $We_{g,cr,0}=11\pm 2$ , indicating that there is a scatter in the results of experimental works; in (Hanson et al., 1963) an even lower value of ~7 is reported. Regarding the dependency between the  $We_{g,cr}$  and  $Oh_l$  numbers (the two most influential), this is generally expressed through the empirical equation 1, where *C* and *n* are fitting coefficients:

$$\frac{We_{g,cr}}{We_{g,cr,0}} = 1 + C \cdot Oh_l^n \tag{1}$$

A list of the coefficients *C*, *n* which were determined in past works is given in Table 1. (Brodkey, 1967) and (Gelfand, 1996) obtained these coefficients by fitting experimental data, while (Cohen, 1994) assumed that the energy required for breakup, is that of an inviscid droplet plus the energy required to overcome the viscous dissipation (see details in section 6.3); this resulted in n=1, while the coefficient *C* was determined by fitting experimental data.

74

Table 1: List of the coefficients *C*, *n* of eq. 1 proposed by different sources for the bag
breakup regime.

source	coeff. C	coeff. n	derivation	comments
(Brodkey, 1967)	1.077	1.6	Empir.	<i>Oh</i> <sub>l</sub> <10
(Cohen, 1994)	1-1.8	1	Semi-Anal.	$10 < We_{g,cr,0} < 100$
				-
(Gelfand, 1996)	1.5	0.74	Empir.	Oh <sub>l</sub> <4
			Ĩ	

In (Hsiang and Faeth, 1995) the droplet momentum equation was used and adopting the viscous timescale of (Hinze, 1949) (eq. 14 in section 2.1), they derived equation 2. Assuming an average value of the drag coefficient  $\overline{C_D}$ , they determined the coefficient C (without mentioning its value) by comparing against experimental data and the model performance was very good.

$$\frac{We_{g,cr}}{We_{g,cr,0}} = \frac{1}{4} \left( 1 + C \cdot \frac{\overline{C_D}}{\sqrt{\varepsilon \cdot We_{g,cr,0}}} Oh_l \right)^2$$
(2)

83

Another approach for the estimation of the critical  $We_g$  number, is to assume that the breakup is ought to Rayleigh-Taylor (R-T) instabilities as in (Zhao et al., 2011) and (Yang et al., 2017). According to this model, when the droplet deformation (usually the cross-stream diameter) exceeds the critical wavelength of the R-T instability (which depends on liquid properties and droplet acceleration), then breakup occurs. The resulting equation (e.g. in (Zhao et al., 2011)) has the form of eq. 3, where *C* is an adjustable coefficient, in the range 1.18-1.48.

$$\left(\frac{We_{g,cr,0}}{We_{g,cr}}\right)^{1/2} + C\left(\frac{Oh_l^2}{We_{g,cr}}\right)^{1/3} = 1$$
(3)

The concept of R-T instabilities has been considered as the main mechanism for breakup in other works as in (Joseph et al., 1999),(Theofanous and Li, 2008), (Theofanous et al., 2012). The group of Prof. Theofanous considered also a different characterization of breakup, with Rayleigh-Taylor piercing (RTP) happening at lower  $We_g$  numbers and shear-induced entrainment (SIE) above a transition  $We_g$ . Generally,

the aforementioned correlations are in qualitative agreement between them, but they do not give insight into the effects of  $Re_g$  and  $\varepsilon$  numbers

98 Turning now to the effect of the  $Re_g$  number and density ratio  $\varepsilon$ , this has not been in 99 detail examined in experimental works due to technical limitations in obtaining low  $Re_g$  and  $\varepsilon$  numbers. On the other hand, their effect has been examined in a few 100 101 numerical works but without providing correlations similar to the aforementioned for 102 the  $Oh_l$  number (e.g. as in eq. 1). As a general remark, they have all concluded that the critical  $We_g$  number increases for low  $Re_g$  and  $\varepsilon$  numbers. More specifically, 103 104 (Aalburg, 2002) found that there is no effect on breakup for  $Re_g>100$  and  $\varepsilon>32$ . 105 Nevertheless, their numerical model could not predict the actual breakup and they 106 assumed that breakup happens when the cross-stream deformation exceeds 60%; 107 despite this limitation, they were able to reproduce the breakup map of (Hsiang and 108 Faeth, 1995). In (Han and Tryggvason, 2001) the authors examined low density ratios 109 ( $\varepsilon$ <10) and found that the  $Re_g$  effect is minimal for  $Re_g$ >200, while decreasing the  $Re_g$ 110 and keeping the other parameters constant can lead to different breakup modes. A 111 similar conclusion was also drawn when the density ratio decreases and approaches 112 unity. In (Jing and Xu, 2010) it is stated that shear breakup is observed only for  $\varepsilon$ >100, while for  $Re_g$  numbers in the range 10<sup>2</sup> up to 10<sup>6</sup> there are slight differences in 113 114 the topology of the bag and the rim. Regarding the effect of density ratio they found 115 different breakup modes for  $\varepsilon = 10$  and 1000 (forward bag and sheet-thinning 116 respectively for  $We_g=27.5$ ) and also significantly lower droplet acceleration and 117 displacement as the density ratio increases. Recently, (Yang et al., 2016) used a 3D model to study breakup at highly unstable conditions ( $Re_g \sim 10^4$ ) and found that 118 119 breakup is affected even for  $\varepsilon > 32$  (the limit proposed by (Aalburg, 2002)), and a 120 lower density ratio results in a higher deformation rate but less intensive 121 fragmentation. Finally, (Kékesi et al., 2014) examined various combinations of  $Re_g$ 122 and  $\varepsilon$  numbers (generally low values) and identified new breakup regimes that have 123 not been observed in experiments.

124 The aim of the present work is to provide a simple but reliable methodology to relate the critical  $We_g$  number with all the actual dimensionless numbers affecting droplet 125 126 breakup, as there is a lack of such a model in literature. In the text follows there is a 127 description of the methodology and then the model results are presented. In the 128 appendix, the derivation of correction factors for the effect of  $Re_g$  number and density 129 ratio is presented along with a correlation to predict the breakup initiation time. 130 Finally in the appendix, the present methodology is related to a modified version of 131 the energy approach of (Cohen, 1994), showing that both concepts are equivalent.

132

# 133 **2 Methodology**

## 134 2.1 Forces and dimensionless numbers

Before proceeding to the presentation of the methodology adopted in the present
work, it is essential to discuss the forces acting on the droplet and the dimensionless
numbers describing droplet breakup.

138 The main forces controlling droplet breakup are the aerodynamic forces induced from

139 the gas phase  $(\sim \rho_g U_g^2 D^2)$ , the surface tension forces  $(\sim \sigma D)$ , the gas viscosity forces

140  $(\sim \mu_a U_a D)$  and the liquid viscosity forces  $(\sim \mu_l U_l D)$ . In the latter case, the liquid

141 velocity  $U_l$  appearing can be estimated from (Hinze, 1955), (Hsiang and Faeth, 1992) 142 as:

$$U_l = \sqrt{\frac{\tau}{\rho_l}} = \sqrt{\frac{\rho_g U_g^2}{\rho_l}} = \frac{U_g}{\sqrt{\varepsilon}}$$
(4)

143 , where  $\varepsilon = \rho_l / \rho_g$  is the density ratio and  $\tau$  denotes stress. This equation implies that 144 gas and liquid inertia forces are essentially equal to one another  $(\rho_l U_l^2 = \rho_g U_g^2)$ . 145 Turning now to the definition of the dimensionless numbers, these are derived by 146 combing different types of forces:

$$We_g \sim \frac{gas \ inertia \ forces}{surface \ tension \ forces} = \frac{\rho_g U_g^2 D^2}{\sigma D} = \frac{\rho_g U_g^2 D}{\sigma}$$
(5)

$$Oh_{l} \sim \frac{liquid \ viscous \ forces}{\sqrt{(inertia \ \cdot \ surface \ tension) \ forces}} = \frac{\mu_{l} U_{l} D}{\sqrt{\rho_{l} U_{l}^{2} D^{2} \cdot \sigma D}}$$
(6)  
$$= \frac{\mu_{l}}{\sqrt{\sigma D \rho_{l}}}$$

$$Re_{g} \sim \frac{gas \ inertia \ forces}{gas \ viscous \ forces} = \frac{\rho_{g} U_{g}^{2} D^{2}}{\mu_{g} U_{g} D} = \frac{\rho_{g} U_{g} D}{\mu_{g}} \tag{7}$$

147 Among them, the  $We_g$  and the  $Oh_l$  numbers are the most influential in droplet 148 breakup, while one can notice that the  $Oh_l$  number despite its wide use and 149 importance, it has a rather strange physical meaning by relating the liquid viscous 150 forces with the square root of inertia times surface tension forces.

151 Using different combinations of the aforementioned forces, one can define additional

152 dimensionless numbers, such as the liquid and gas Capillary numbers ( $Ca_l$  and  $Ca_g$ ),

153 the liquid *Re* number (*Re*<sub>*l*</sub>) and the gas-liquid *Re* number (*Re*<sub>*g*/*l*</sub>):

$$Ca_{l} \sim \frac{liquid \ viscous \ forces}{surface \ tension \ forces} = \frac{\mu_{l} U_{l} D}{\sigma D} = \frac{\mu_{l} U_{g}}{\sigma \sqrt{\varepsilon}}$$
(8)

$$Ca_g \sim \frac{gas \ viscous \ forces}{surface \ tension \ forces} = \frac{\mu_g U_g D}{\sigma D} = \frac{\mu_g U_g}{\sigma}$$
<sup>(9)</sup>

$$Re_{l} \sim \frac{liquid\ inertia\ forces}{liquid\ viscous\ forces} = \frac{\rho_{l}U_{l}^{2}D^{2}}{\mu_{l}U_{l}D} = \frac{\rho_{l}U_{g}\ D}{\mu_{l}\sqrt{\varepsilon}} = Re_{g}\frac{\sqrt{\varepsilon}}{N} = \frac{\sqrt{We_{g}}}{Oh_{l}}$$
(10)

$$Re_{g/l} \sim \frac{gas \ inertia \ forces}{liquid \ viscous \ forces} = \frac{\rho_g U_g^2 D^2}{\mu_l U_l D} = \frac{\sqrt{\rho_g \rho_l} U_g \ D}{\mu_l} = Re_g \frac{\sqrt{\varepsilon}}{N}$$
(11)

The gas-liquid Re number  $(Re_{g/l})$  and the liquid Re number  $(Re_l)$  is proved to represent 154 the same quantity. Both of them are equal to  $Re_g\sqrt{\epsilon}/N$  or  $\sqrt{We_g}/Oh_l$ ; the latter was 155 used in (Aalburg, 2002) to develop a new breakup map as it was proved to dominate 156 157 the breakup at large  $Oh_l$  numbers. The gas-liquid Re number ( $Re_{g/l}$ ) has also appeared in the work of (Schmehl, 2002), named there as "deformation" Re number. Finally, 158 the term  $N/\sqrt{\varepsilon}$  in equations 10 and 11 depends on the physical properties and has 159 160 appeared in (Gelfand, 1996), (Aalburg, 2002), while in (Kékesi et al., 2014) it was also used to develop a new breakup map along with the  $Re_g$  number. Among the 161 162 aforementioned new dimensionless numbers, the  $Ca_l$  number will be proved in the 163 subsequent sections to be the most valuable one and it is related to the other numbers 164 with the following equation:

$$Ca_{l} = \frac{\mu_{l} U_{g}}{\sigma \sqrt{\varepsilon}} = Oh_{l} \sqrt{We_{g}} = \frac{We_{g}}{Re_{l}}$$
(12)

Finally, for the non-dimensionalization of time, the shear breakup timescale of (Nicholls and Ranger, 1969) is widely used (eq. 13), which in fact represents the liquid convection timescale. For large  $Oh_l$  numbers, the viscous timescale of (Hinze, 169 1949) has also been used (eq. 14)

$$t_{sh} = \frac{D}{U_l} = \frac{D\sqrt{\varepsilon}}{U_g} \tag{13}$$

$$t_{vis} = \frac{\mu_l}{\rho_g U_g^2} = t_{sh}/Re_l \tag{14}$$

170

#### 171 **2.2 Total Force approach**

As mentioned in the previous section 2.1, there are various types of forces acting on the droplet. One can group them into forces that tend to deform the droplet ( $F_{DEF}$ ) and forces tending to restore the droplet ( $F_{RES}$ ) in its original shape, or equivalently into forces from the gas side ( $F_{gas}$ ) and forces from the liquid side ( $F_{liq}$ ). These two types of forces are overall calculated as in equations 15 and 16,

$$F_{DEF/gas} = \rho_g U_g^2 D^2 - C_{vis,g} \mu_g U_g D \tag{15}$$

$$F_{RES/liq} = \sigma D + C_{vis,l} \mu_l U_l D \tag{16}$$

177 , where the terms  $C_{vis,g}$  and  $C_{vis,l}$  are adjustment factors aiming to reveal the 178 contribution of the gas and liquid viscous forces correspondingly on the evolution of 179 the phenomenon. For convenience here, the gas viscous forces (which are restorative) 180 appear in the deformation forces but with a negative sign. Thus, the term  $F_{DEF/gas}$ 181 represents the net deformation forces from the gas side. 182 The ratio of these forces is called here *TFR* (Total Force Ratio) and it is shown in eq. 183 17, in which the liquid velocity  $U_l$  has been replaced with the corresponding gas terms 184 according to eq. 4:

$$TFR = \frac{F_{DEF/gas}}{F_{RES/liq}} = \frac{\rho_g U_g^2 D^2 - C_{vis,g} \mu_g U_g D}{\sigma D + C_{vis,l} \mu_l \frac{U_g}{\sqrt{\varepsilon}} D}$$
(17)

185 Diving both forces with  $\sigma D$  (the surface tension forces) and after some manipulation 186 of eq. 17 we can reach the following equation 18, where  $f_{vis,g}$  represents a correction 187 factor for the gas viscosity effects.

$$TFR = \frac{We_g}{f_{vis,g} \left(1 + C_{vis,l} \cdot Ca_l\right)}$$
(18)

$$f_{vis,g} = \frac{1}{1 - C_{vis,g}(1/Re_g)} \tag{19}$$

188

As seen, the *TFR* is in fact the  $We_g$  number divided/corrected by two terms (both higher than unity) to account for viscosity effects. In the limit of inviscid flow, *TFR* is simply the  $We_g$  number and a close physical approximation of this situation corresponds to conditions characterized by low  $Oh_l$  and high  $Re_g$  numbers.

The model proposed in this study, assumes that there is a critical *TFR* value (*TFR*<sub>cr</sub>), above which, breakup occurs (or there is generally transition among the different breakup modes). It is further assumed that the critical *TFR* value depends only on the breakup mode (bag, sheet-thinning etc) and not on other dimensionless numbers (e.g. the *Oh*<sub>l</sub> number as in the case of  $We_{g,cr}$ ), since by definition *TFR* accounts for all types of forces. This critical value pertains to the  $We_{g,cr,0}$  value, which depends only on the breakup mode and it is generally known from experiments ( $We_{g,cr,0}$  was defined in the introduction for low  $Oh_l$  and high  $Re_g$  numbers).

201 Nevertheless, there is also one parameter that has not been yet included in the present

shown that the critical  $We_g$  number increases for low  $\varepsilon$  values, thus the  $We_{g,cr,0}$  has to

analysis. This is the density ratio  $\varepsilon$ . Past works (presented in the introduction) have

- 204 be multiplied by a correction factor  $f\varepsilon$  ( $f\varepsilon$ >1) to account for low density ratio effects.
- 205 Thus the final criterion for breakup should be defined as  $TFR_{cr}=We_{g,cr,0} \cdot f_{\varepsilon}$ .

202

206 Replacing the  $TFR_{cr}$  from eq. 18, the following equations 20-23 describe the relation 207 among  $We_{g,cr}$  and the rest dimensionless numbers.

$$\frac{We_{g,cr}}{We_{g,cr,0}} = f_{\varepsilon} \cdot f_{vis,g} \cdot f_{vis,l}$$
(20)

$$f_{\varepsilon} = 1 + C_{\varepsilon} \frac{1}{\varepsilon}$$
<sup>(21)</sup>

$$f_{vis,g} = \frac{1}{1 - C_{vis,g} (Re_g)^{-ng}}$$
(22)

$$f_{vis,l} = 1 + C_{vis,l} \cdot (Ca_l)^{nl} \tag{23}$$

The density correction factor  $f\varepsilon$  is given by equation 21 with  $C_{\varepsilon}=3$  (see section 6.1.2 for details), while the gas and liquid viscosity correction factors are re-written in equations 22 and 23 in a more generic way (using the exponents ng, nl) to account for deviations from the preceding theoretic analysis (theoretically it is ng=nl=1). 212 Regarding the adjustable coefficients  $C_{vis,g}$  and ng for the effect of gas viscosity in eq. 213 22, these were determined by performing numerical simulations (see section 6.1.1 for 214 details) and found to be equal to  $C_{vis,g}=55$  and ng=1.1, following a best fitting 215 algorithm, which is close to the estimated value of 1. Regarding the liquid viscosity 216 coefficients, these were depending on the breakup mode and were estimated to be in 217 the range  $C_{vis,l}=0.06 - 0.26$  and nl=0.9 - 1.0 (close to the theoretic value of 1); nevertheless, a value of *nl*=1 was used throughout this study for all breakup modes. 218 219 These were initially determined based on the breakup boundaries of (Hsiang and 220 Faeth, 1995) and then fine-tuned using the experimental and numerical data shown in 221 sections 3.2.2 and 3.2.3.

222 The values used for the adjustable coefficients  $C_{vis,g}$ ,  $C_{vis,l}$ , ng, nl and  $C_{\varepsilon}$  are given in 223 Table 2, as well as the  $We_{g,cr,0}$  value; the catastrophic breakup regime is also included, 224 but it has been estimated without having a sufficient amount of data. All these 225 coefficients are assumed, for the current status of work, to be constant numbers but it 226 is likely, that they are functions of additional numbers (e.g the density ratio), or there 227 are interdependencies between them. It has also to be noted, that all coefficients were assumed to be unaffected by the breakup mode, except of the  $C_{vis,l}$  coefficient which is 228 229 the most influential.

- 230
- Table 2: Values of the adjustable coefficients  $C_{vis,g}$ , ng,  $C_{vis,b}$ , nl,  $C_{\varepsilon}$  used in equations 232 21-23. The  $We_{g,cr,0}$  value is also shown.

Breakup mode  $We_{g,cr,\theta}$   $C_{vis,g}$  ng  $C_{vis,l}$  nl  $C_{\varepsilon}$ 

bag	10	55	1.1	0.26	1.0	3
transitional	16	55	1.1	0.20	1.0	3
Sheet-thinning	63	55	1.1	0.06	1.0	3
catastrophic	350	55	1.1	0.01	1.0	3

A graphical representation of the aforementioned correction factors is shown in Fig.1, according to which liquid viscosity effects become important for  $Ca_l>0.5$ , gas viscosity effects for  $Re_g<300$  and density ratio effects for  $\varepsilon<20$ .

237



238

Fig.1: Correction factors for the effect of  $Ca_l$  (for bag breakup),  $Re_g$  and density ratio 240  $\varepsilon$ .

241

A final comment has to be made as concerns the methodology described in thissection. It represents an extension of the experimental observations for the dominant

role that  $We_g$  number plays on distinguishing and controlling breakup regimes and it 244 245 is not based on a physical principle, such as the momentum conservation equation or 246 the deformation of the droplet beyond a threshold (e.g. the R-T wavelength). 247 Nevertheless, in the appendix (section 6.3) it is proved that the model equations are equivalent to those obtained by using a modified version of the energy approach by 248 249 (Cohen, 1994). As it will be shown in the following sections, the present model 250 provides with sufficient accuracy a unified criterion to predict the breakup outcome 251 for any combination of  $We_g$ ,  $Ca_l$  (or  $Oh_l$ ),  $Re_g$  and  $\varepsilon$  numbers.

252

# 253 **3 Results and discussion**

#### 254 **3.1 Qualitative model performance**

In this section the qualitative model performance is examined by using equations 20-23 and adopting some reference values for the  $Re_g$  number and density ratio  $\varepsilon$  (equal to 1000 for both) to calculate the correction factors  $f_{vis,g}$  and  $f_{\varepsilon}$ . Except of the classical  $We_g - Oh_l$  breakup map, alternative breakup maps in the  $We_g - Re_{l/g}$  and  $We_g - Ca_l$ planes are also presented.

260 **3.1.1 The**  $We_g - Oh_l$  plane

In order to reproduce the  $We_g - Oh_l$  plane, the  $Ca_l$  number in eq. 23 is replaced with  $Ca_l = Oh_l \sqrt{We_g}$  (see eq. 12). Using these modifications and setting nl=1, eq 20 is transformed into:

$$\frac{We_{g,cr}}{We_{g,cr,0}} = f_{\varepsilon} \cdot f_{vis,g} \cdot \left(1 + C_{vis,l} \sqrt{We_g} \cdot Oh_l\right)$$
(24)

This is a quadratic equation in respect to  $\sqrt{We_g}$  having two roots. Keeping only the positive one, the final expression for the dependency of  $We_g$  versus  $Oh_l$  is given in equation 25.

$$We_{g,cr} = \frac{1}{4} \left[ \left( C_{vis,l} \cdot We_{g,cr,0} \cdot f_{\varepsilon} \cdot f_{vis,g} \cdot Oh_{l} \right) + \sqrt{\left( C_{vis,l} \cdot We_{g,cr,0} \cdot f_{\varepsilon} \cdot f_{vis,g} \cdot Oh_{l} \right)^{2} + 4We_{g,cr,0} \cdot f_{\varepsilon} \cdot f_{vis,g}} \right]^{2}$$

$$(25)$$

The model results for the bag breakup mode ( $We_{g,cr,0}$ , =10) are shown in Fig.2 along with the corresponding correlations from similar referenced works. As it can be seen, the present model can capture the qualitative behaviour of the dependency between  $We_{g,cr}$  and  $Oh_l$ , while it is very close to the results of (Hsiang and Faeth, 1995). Similar agreement has been achieved for the transitional and the sheet-thinning breakup regimes, using the adequate coefficients  $C_{vis,l}$ .



273

Fig.2: Results of the present model for the bag breakup regime in the  $We_g - Oh_l$  plane. The corresponding results from other correlations are also shown.

277 Regarding the effect of  $Re_g$  number and density ratio on the critical  $We_g$  number, this 278 is shown in Fig.3 for the bag breakup case ( $We_{g,cr,0}=10$ ), which is representative for all 279 breakup modes. As seen, decreasing the  $Re_g$  and  $\varepsilon$  numbers results in a slight increase 280 of the critical  $We_g$  number. This is in accordance with the findings of past works 281 presented in the introduction.



Fig.3: (a) effect of Re number, (b) effect of density ratio on the bag breakupboundary.

285

Regarding the asymptotic behavior of eq. 24 for large *Oh* numbers, the product  $C_{vis,l}\sqrt{We_g} \cdot Oh_l$  is much higher than unity, thus equation 24 becomes  $\sqrt{We_g}/Oh_l =$   $f_{\varepsilon} \cdot f_{vis,g} \cdot C_{vis,l} \cdot We_{g,cr,0}$ , which is a constant number. This is in accordance with the findings of (Aalburg, 2002) and (Zhao et al., 2011); the first one proved this by performing numerical simulations and the second one by using the R-T instabilities theory.

#### 293 **3.1.2** Alternative breakup planes

Alternative breakup planes can be developed by using directly eq. 23 (for the  $We_g$  –  $Ca_l$  plane) or by replacing the  $Ca_l$  number in eq. 23 with  $Ca_l = We_g/Re_{g/l}$  (from eq. 12) in order to develop the  $We_g - 1/Re_{g/l}$  plane; after some manipulation, the resulting equation is eq. 26. As in the previous case, the coefficient *nl* in eq. 23 has been set equal to 1.

$$\frac{We_{g,cr}}{We_{g,cr,0}} = \frac{f_{\varepsilon} \cdot f_{vis,g}}{1 - f_{\varepsilon} \cdot f_{vis,g} \cdot C_{vis,l} \frac{1}{Re_{g/l}} We_{g,cr,0}}$$
(26)

299 The planes  $We_g - Ca_l$  and  $We_g - 1/Re_{g/l}$  are plotted in Fig.4a, b respectively by using 300 the same coefficients as in section 3.1.1 for the  $We_g - Oh_l$  plane. All planes presented 301 so far look similar to one another, but there is a substantial difference in the  $We_g$  – 302  $1/Re_{g/l}$  plane. In this plane based on eq. 26 there is a critical condition for breakup, i.e  $1/Re_{g/l} < 1/(f_{\varepsilon} \cdot f_{vis,g} \cdot C_{vis,l} \cdot We_{g,cr,0})$ . This means that breakup is not always 303 observed for high  $1/Re_{g/l}$  numbers. This contradicts the results deduced from the  $We_g$ 304 305  $-Oh_l$  and  $We_g - Ca_l$  planes in which there is no limitation for breakup. For the time being, there are no experimental data examining extremely high values of  $\sqrt{We_q}/Oh_l$ 306 307 (or  $We_g/Ca_l$ , or  $1/Re_{g/l}$ ), thus a clear suggestion for the most appropriate breakup 308 plane, cannot be given.



Fig.4: Results of the present model in (a) the  $We_g - Ca_l$  plane and (b) the  $We_g - 1/Re_{g/l}$ plane.

312

313 Among the breakup planes presented so far, our opinion is that the most suitable is the  $We_g - Ca_l$  plane, since its axes represent gas inertia versus liquid viscous forces, both 314 315 non-dimensionalised with the same quantity, i.e the liquid surface tension forces, 316 while the asymptotic behavior at large  $We_g/Ca_l$  values agrees with the one predicted 317 by (Aalburg, 2002) and (Zhao et al., 2011). Furthermore, there is an explicit relation 318 between  $We_g$  and  $Ca_l$  for any value of the coefficient nl, while for the other numbers 319  $(Oh_l \text{ or } Re_{g/l})$  there is an implicit relation with the  $We_g$  number when nl is not unity. 320 For the aforementioned reasons, the  $We_g - Ca_l$  plane is further used in this work.

321

#### 322 **3.2** Comparison against experimental and numerical data

In this section, a large amount of experimental and numerical data are superimposed in the proposed  $We_g - Ca_l$  plane to reveal the model capabilities compared to other works. It is of importance to highlight that the  $Re_g$  number and the density ratio are

not predefined by assuming reference values as in section 3.1, but they are explicitly 326 327 calculated. The results presented here have been grouped according to the breakup 328 outcome into a) non-breakup, b) bag breakup, c) transitional, d) sheet-thinning and 329 finally e) catastrophic regimes. The transitional breakup regime includes the 330 intermediate regimes bag-stamen, dual-bag, multi-bag and plume-shear for reasons of 331 simplicity and clearness. For reasons of distinctness and readability, the experimental 332 data and the numerical data are discussed in separate sections. Prior to the 333 presentation of the results, the concept of the effective  $We_g$  number, is introduced.

334

#### 335 3.2.1 The effective We number

In order to avoid using multi-dimensional graphs (or 2-dimensional planes with parametric curves as in Fig.3) for the cases in which different  $Re_g$  numbers or density ratios are examined, equation 20 is rearranged and the  $We_g$  number is replaced with an effective  $We_g$  number ( $We_{g,eff}$ ), which takes into consideration the secondary effects of  $Re_g$  number and density ratio on breakup outcomes. This is numerically represented in eq. 27:

$$\frac{We_{g,eff}}{We_{g,cr,0}} = 1 + C_{vis,l} \cdot (Ca_l)^{nl}, \qquad We_{g,eff} = \frac{We_g}{f_{\varepsilon} \cdot f_{vis,g}}$$
(27)

For example, in a case with  $We_g=13$ ,  $Re_g=70$  and a density ratio equal to 10, the effective  $We_g$  number is:

$$We_{g,eff} = \frac{13}{(1+3/10) \cdot (1-55 \cdot 70^{-1.1})^{-1}} = \frac{13}{1.33 * 2.04} = 4.79$$

and probably the droplet will not breakup, since it is much lower than  $We_{g,cr,0}=10$ . On the other hand, in a case with large  $Re_g$  and density ratio (e.g 8000 and 1000 respectively),  $We_{g,eff}$  is equal to 12.93, close to the normal  $We_g$  number of 13. Therefore, it is better and more straightforward for droplet breakup characterization, the  $We_{g,eff}$  instead of the  $We_g$  number to be used. In the appendix (section 6.2), the effective  $We_g$  number is also used to predict the breakup initiation time.

350

#### 351 **3.2.2 Comparison against experimental data**

352 The experimental data used to assess the model performance are presented separately 353 according to the experimental technique used, i.e the shock tube and the continuous 354 air jet. For the shock tube experiments (denoted as ST), there are 46 experimental points obtained from the works of (Hanson et al., 1963), (Hirahara and Kawahashi, 355 1992), (Hsiang and Faeth, 1995), (Dai and Faeth, 2001), while for the continuous air 356 357 jet experiments (CAJ), there are 101 experimental points obtained from the works of 358 (Krzeczkowski, 1980),(Arcoumanis et al., 1994), (Liu and Reitz, 1997), (Lee and 359 Reitz, 2000), (Zhao et al., 2010), (Opfer et al., 2012), (Flock et al., 2012), (Jain et al., 360 2015). The results of the present model are shown in Fig.5(a) and (b) for both the experimental techniques (ST and CAJ respectively). 361





Fig.5: Results of the present model in the  $We_{g,eff} - Ca_l$  plane for (a) Shock Tube and (b) Continuous Air Jet experiments.

As seen, the fitting of the experimental data is generally good, especially for the CAJ 366 367 experiments with an exception for one experimental point of (Flock et al., 2012) in the 368 sheet-thinning regime, which was observed at a small  $We_g$  number of 32, rather corresponding to the transitional regime; nevertheless, in the experimental photos of 369 370 this case, the sheet formation was clear. Also the experiments by Reitz and coworkers (Liu and Reitz, 1997), (Lee and Reitz, 2000) at  $We_g=54$  were considered as 371 372 "bag" in the relevant paper, but from their experimental photos it seems rather to 373 undergo a multi-bag breakup; thus in the present paper they were included in the 374 "transitional" regime. Regarding the ST experiments, there is a scattering in the 375 transitional breakup regime in which there are some cases (5 from (Hanson et al., 376 1963) and 1 from (Hirahara and Kawahashi, 1992)) characterized by a relatively low 377 We number of 7-8 which exhibit bag-stamen breakup regime. Nevertheless, it is not always clear what someone considers as bag or bag-stamen, while other parameters 378 379 such as the Mach number and turbulence levels may affect the breakup outcome. Such

380 secondary controlling physical parameters have not been considered in the present381 model.

In relevance to the breakup map of (Hsiang and Faeth, 1995), the boundary of transitional breakup appears for lower values of  $We_g$  number, and includes the bagstamen, dual-bag, bag-plume, shear plume breakup regimes. The determination of this regime was mainly based on the experiments of (Zhao et al., 2010), which are more recent than the experiments of (Hsiang and Faeth, 1995). One should recall also, that these two works use a different experimental technique.

388

#### 389 3.2.3 Comparison against numerical data

390 In this section the model performance is compared against numerical 2D 391 axisymmetric simulations. The numerical data used to assess the model performance 392 are 66 simulations performed in the past from the authors' group in (Strotos et al., 393 2016a, b; Strotos et al., 2016c), as well as simulations performed in the current work (see appendix), and 43 simulations from (Han and Tryggvason, 2001). For reasons of 394 395 readability these are presented in different graphs, i.e. in Fig.6 (a) and (b) 396 respectively. The "forward bag" observed in (Han and Tryggvason, 2001) was 397 included in the transitional regime here. In these simulations the  $Re_g$  number was in 398 the range 50 - 4000 and the density ratio in the range 5 - 800, which means that there 399 are cases (those with low  $Re_g$  and  $\varepsilon$ ) in which the effective  $We_{g,eff}$  number differs 400 significantly among them compared to using the classical  $We_g$  number. This is an 401 additional reason, why the use of the effective  $We_g$  number is proposed as more

402 representative for such types of droplet breakup characterization, compared to the403 standard one.



405 Fig.6: Results of the present model in the  $We_{g,eff} - Ca_l$  plane for (a) simulations of the 406 authors' group and (b) simulations of (Han and Tryggvason, 2001).

407

404

408 Based on the graphs, the overall model performance towards separating the various 409 breakup regimes is good and only a few exceptions seem to deviate from the proposed 410 breakup boundaries. In the authors' group simulations, there are two cases which 411 breakup but appear in the non-breakup region of the map, whilst in the (Han and 412 Tryggvason, 2001) simulations, there are 5 bag breakup cases which appear in the 413 transitional region of the map. Nevertheless, in all these cases (characterized by low 414  $Re_g$  numbers and density ratios) the breakup modes differ from those observed in the 415 experiments and it is a matter of convention what someone considers as transitional 416 breakup. Furthermore, the breakup phenomenon is a continuous process (as stated in 417 (Guildenbecher et al., 2009)) and there is not yet a deterministic single criterion for 418 the transition among different breakup regimes. Based on their recommendation a 419 zone rather than a single line should be used to separate the breakup regimes.

However, the present work offers the introduction of an alternative set of parameters for visualizing the transition of droplet breakup mechanisms, which seems to be more representative and close to reality compared to previous work and in that respect should be considered as a step-forward towards understanding the underling physics represented by more correct variables.

425

# 426 **4** Conclusions

427 In the present work, a new proposed total force approach has been used to determine 428 the dependency of the critical  $We_g$  number ( $We_{g,cr}$ ) separating different breakup 429 regimes on all other non-dimensional numbers ( $Re_g$ ,  $\varepsilon$  and  $Oh_l$  or  $Ca_l$ ). According to 430 this approach, the breakup phenomenon is controlled by the ratio of the sum of the 431 deformation versus the sum of restorative forces; for negligible viscosities, this ratio 432 reduces to the classical  $We_g$  number. Breakup (or generally transition between 433 breakup regimes) occurs when this ratio exceeds a critical value; the latter is equal to 434 the critical  $We_g$  number corresponding to low  $Oh_l$  numbers (termed here as  $We_{g,cr,0}$ ) and it is known from experimental data. 435

The proposed model includes adjustable coefficients, which were determined by performing numerical simulations and comparing against a large amount of experimental and numerical data found in literature. Overall, a good qualitative and quantitative agreement has been achieved. To unify cases with different conditions (namely  $Re_g$  and  $\varepsilon$  numbers) an effective  $We_g$  number ( $We_{g,eff}$ ) was proposed. This is essentially the classical  $We_g$  number, corrected by two factors which account for the secondary effects of  $Re_g$  and  $\varepsilon$  numbers. The model results were presented in a new breakup map, the  $We_{g.eff} - Ca_l$  plane; using the  $Ca_l$  number instead of the  $Oh_l$ , corresponds directly to the relation of gas inertia versus liquid viscosity when both are non-dimensionalised using the same quantity (the surface tension forces), while using the  $We_{g.eff}$  instead of the  $We_g$  number, enables the inclusion of additional parameters in the same plane. The effective  $We_{g.eff}$  number was also used to predict the breakup initiation time, shown in the appendix

449 The present methodology is not derived from physical principles, such as the 450 momentum equation or the Rayleigh-Taylor instabilities. It is rather an extension of 451 experimental observations and numerical data towards including in a unified way all 452 possible interdependencies among the forces acting on a droplet. Nevertheless, it is 453 shown in the appendix that this model is fully compatible with an energy approach relating the required kinetic energy for breakup with that of an inviscid droplet. The 454 455 methodology proposed applies for Newtonian fluids, in laminar, isothermal and 456 incompressible flow conditions.

457

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# 462 6 Appendix

## 463 6.1 Derivation of correction factors

464 In this section, the 2D axisymmetric simulations performed for the determination of 465 the correction factors  $f_{vis,g}$  and  $f_{\varepsilon}$  are presented. To determine these factors, all 466 parameters were kept constant and only one was changing each time to reveal the 467 effect of  $Re_g$  number and density ratio; the reference settings used were  $Ca_l=0.03$ ,  $Re_g$ =400 and  $\varepsilon$ =800. The cases examined were 55 and 31 of them are presented in 468 469 detail in Table 3. The VOF methodology (Hirt and Nichols, 1981) has been used and 470 implemented in ANSYS FLUENT v16.1 (ANSYS®FLUENT, 2015); details on the 471 methodology used can be found in earlier authors' work mentioned in section 3.2.3. 472 Note also that here, only the breakup outcome is presented, grouped into "breakup", "no breakup" and "marginal", with the latter representing cases with an unclear 473 474 breakup outcome; more details on the droplet shapes and physical mechanisms are 475 going to be published in a separate article.

Table 3: List of the physical parameters of selected cases for the determination of thecorrection factors.

Weg	Reg	Ohı	Ca <sub>l</sub>	ε	N
25	50.0	0.006	0.03	800	1.70
30	50.0	0.005	0.03	800	1.41
30	70.0	0.005	0.03	800	1.98
14	100.0	0.008	0.03	800	6.06
16	100.0	0.008	0.03	800	5.30
20	100.0	0.007	0.03	800	4.24
30	100.0	0.005	0.03	800	2.83
12	200.0	0.009	0.03	800	14.14

Weg	Reg	Oh,	Caı	ε	N
13	200.0	0.008	0.03	800	13.05
14	200.0	0.008	0.03	800	12.12
11	400.0	0.009	0.03	800	30.86
11	400.0	0.009	0.03	800	30.86
11	400.0	0.009	0.03	800	30.86
12	400.0	0.009	0.03	800	28.28
12	400.0	0.009	0.03	800	28.28
12	400.0	0.009	0.03	800	28.28
11	2400.0	0.009	0.03	800	185.13
12	400.0	0.009	0.03	100	10.00
13	400.0	0.008	0.03	20	4.13
14	400.0	0.008	0.03	20	3.83
16	400.0	0.008	0.03	10	2.37
16	400.0	0.008	0.03	5	1.68
20	400.0	0.007	0.03	5	1.34
20	400.0	0.007	0.03	3	1.04
20	400.0	0.007	0.03	2	0.85
14	400.0	0.160	0.6	800	484.87
20	400.0	0.671	3	800	1697.06
18	400.0	1.414	6	800	3771.24
25	400.0	1.200	6	800	2715.29
40	400.0	3.953	25	800	7071.07
60	400.0	3.227	25	800	4714.05

#### 480 6.1.1 Effect of gas viscosity

481 The effect of gas viscosity (i.e the  $Re_g$  number) on droplet breakup for  $Ca_l=0.03$ ,  $\varepsilon$ =800 is presented in Fig.7 in a  $We_g - Re_g$  plane. The curve representing the limiting 482 condition for breakup is  $11.1 \cdot (1-55 \cdot Re^{-1.1})^{-1}$ , while the corresponding curve 483 484 representing the data of (Han and Tryggvason, 2001) for  $\varepsilon = 10$  is also shown. As seen, 485 the present results are in qualitative agreement with those of (Han and Tryggvason, 486 2001) despite the fact that the density ratios are different; additional simulations are 487 required to investigate possible dependency on the density ratio and the  $Ca_l$  (or  $Oh_l$ ) number. 488



489

490 Fig.7: Effect of gas viscosity ( $Re_g$  number) on droplet breakup for  $Ca_l=0.03$ ,  $\varepsilon=800$ . A 491 curve representing the corresponding results of (Han and Tryggvason, 2001) for  $\varepsilon=10$ , 492 is also shown.

#### 494 **6.1.2 Effect of density ratio**

495 The effect of density ratio on droplet breakup for  $Ca_1=0.03$ , Reg=400 is shown in Fig.8 in a  $We_g - \varepsilon$  plane. The curve representing the limiting condition for breakup is 496 497  $11.5(1+3\cdot1/\epsilon)$  and it is in close agreement with the one representing the data of 498 (Aalburg, 2002) for  $Re_g=50$  and  $Oh_l=0.001$  in which the correction factor was 499 estimated (by the authors of the present work) to be  $exp(2.68/\varepsilon)$ ; possible dependency 500 on the  $Ca_l$  (or the  $Oh_l$ ) number was not examined and additional simulations are 501 required for that. A final comment has to be made for the correction factor  $f\varepsilon = 1 + C_{\varepsilon} \cdot 1/\varepsilon$  used to account for the effect of density ratio. Since the density ratio  $\varepsilon$  is 502 503 not appearing in the TFR number, it was "manually" included in the present analysis. 504 Nevertheless, its form is not arbitrary. It was inspired by the work of (Jalaal and 505 Mehravaran, 2014) who found that the interfacial instabilities on the droplet's surface 506 begin at a  $We_g$  number which is analogous to  $(1+1/\varepsilon)$ .



508 Fig.8: Effect of density ratio on droplet breakup for  $Ca_l=0.03$ , Re=400.

507

## 510 **6.2 Estimation of the breakup initiation time**

The effective  $We_g$  number ( $We_{g,eff}$ ) defined in section 3.2.1 can be used to include the effects of  $Re_g$  number and density ratio on the breakup initiation time. Generally, there is not a clear definition what is meant by the term "initiation" time. Here, breakup initiation time is the instant at which there is droplet detachment or the instant at which the droplet interface is corrupted and holes are created. Analyzing the numerical data used in section 3.2.3, the following equation 28 can be used to predict the breakup initiation time, with less than 20% error (see Fig.9):

$$\frac{t_{break}}{t_{sh}} = 2.87 \left( We_{g,eff} - 8 \right)^{-0.26} (1 + 2.560 h_l^{0.63})$$
(28)

This equation has the same form as the one proposed by (Pilch and Erdman, 1987), but additionally predicts that the breakup time increases with decreasing  $Re_g$  and  $\varepsilon$ numbers. In (Pilch and Erdman, 1987) the dependency of break initiation time versus the  $We_g$  number was analogous to ( $We_g - 12$ )<sup>-0.25</sup> and in (Reinecke and Waldman, 522 1975) proportional to  $(We_g - 8)^{-0.25}$ . Here an exponent of -0.26 has been estimated, 523 which is close to the aforementioned values.

Regarding the overall behavior of eq. 28 in relevance to other correlations based on experimental data, the predicted breakup time is in-between the one predicted by the correlations of (Pilch and Erdman, 1987) and (Dai and Faeth, 2001) for a wide range of  $We_g$  numbers (all others parameters regarded constant), while it predicts a similar effect of  $Oh_l$  number as the one predicted by the correlations of (Pilch and Erdman, 1987),(Hsiang and Faeth, 1992),(Gelfand, 1996). These trends are shown in Fig.10.



530

531 Fig.9: Prediction of breakup initiation time with eq. 28. The error lines of  $\pm 20\%$  are 532 also shown.

533



Fig.10: Prediction of breakup initiation time with eq. 28. (a) effect of  $We_g$ , (b) effect of  $Oh_l$  number. Correlations from other researchers are also shown.

537

# 538 6.3 Relation to Cohen's approach

539 In (Cohen, 1994) it was assumed that the kinetic energy required for breakup is that 540 of an inviscid droplet plus the energy required to overcome the energy dissipated by 541 the liquid viscosity; this is shown mathematically in eq. 29 including also the 542 dissipation in the gas phase.

$$\frac{1}{2}\frac{\pi D^3}{6}\rho_g U_g^2 = \left(\frac{1}{2}\frac{\pi D^3}{6}\rho_g U_g^2\right)_{vis=0} + C_{vis,l}(\mu_l U_l D^2) + C_{vis,g}(\mu_g U_g D^2)$$
(29)

In relevance to Cohen's approach, in the liquid dissipation term he assumed that there is a "mixing velocity"  $U_{mix}$ , which was determined by comparing against experimental data; instead of that here, the liquid phase velocity  $U_l$  is used, along with the adjustable coefficient  $C_{vis,l}$ . Non-dimensionalising eq 29 with the surface energy of the spherical droplet  $\sigma \pi D^2$ , and substituting the liquid velocity from eq. 4, we get equation 30 in which the  $We_g$  number in the limit of inviscid flow ( $We_{g,cr,0}$ ) has appeared in the RHS of the equation.

$$We_g = We_{g,cr,0} + 12 \frac{C_{vis,l}}{\pi} Ca_l + 12 \frac{C_{vis,g}}{\pi} \frac{We_g}{Re_g}$$
(30)

Rearranging eq. 30 and dividing by  $We_{g,cr,0}$  we get eq. 31 which is identical to the equation derived with the total force approach in section 2.2 (with ng, nl,  $f\varepsilon$  equal to unity and including all constants inside the terms  $C_{vis,g}$  and  $C_{vis,l}$ )

$$\frac{We_g}{We_{g,cr,0}} \left( 1 - \left( 12\frac{C_{vis,g}}{\pi} \right) \frac{1}{Re_g} \right) = 1 + \left( 12\frac{C_{vis,l}}{\pi We_{g,cr,0}} \right) Ca_l$$
(31)

#### 7 Nomenclature

Roman symbols				
Symbol	Description	Units		
С	Adjustable coefficient	-		
Ca	Capillary number $Ca = \mu U / \sigma$	-		
D	diameter	m		
f	Correction factor	-		
F	force	Ν		
n,ng,nl	Adjustable exponent			
Oh	Ohnesorge number $Oh = \mu / \sqrt{\rho \sigma D}$	-		
Re	Reynolds number $Re = \rho UD/\mu$	-		
t	time	S		
U	reference velocity	m/s		
We	Weber number $We = \rho U^2 D / \sigma$	-		

# 

# <u>Greek symbols</u> Symbol

Symbol	Description	Units
3	density ratio $\varepsilon = \rho_l / \rho_g$	-
μ	viscosity	kg/ms
N	Viscosity ratio $N = \mu_l / \mu_g$	
ρ	density	kg/m <sup>3</sup>
$\sigma$	surface tension coefficient	N/m

# 

<u>Subscripts</u>

Symbol	Description
0	Reference value
br	breakup
cr	critical
DEF	deformation
eff	effective
g or gas	gas
l or liq	liquid
RES	restore

viscosity vis

#### **Abbreviations**

Description
Continuous Air Jet
Rayleigh-Taylor
Shock tube
Total Force Ratio
Volume of Fluid

560

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