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Numerical investigation of aerodynamic droplet breakup in a high temperature gas environment

George Strotos^{1,a,*}, Ilias Malgarinos^{1,b}, Nikos Nikolopoulos^{1,c}, Manolis Gavaises^{1,d}

¹School of Engineering and Mathematical Sciences, City University London, Northampton Square, EC1V 0HB, London, UK

^a George.Strotos.1@city.ac.uk

^b Ilias.Malgarinos.1@city.ac.uk

^c Nikolaos.Nikolopoulos.1@city.ac.uk

^d M.Gavaises@city.ac.uk

*Corresponding author

Abstract

The Navier-Stokes equations, energy and vapor transport equations coupled with the VOF methodology and a vaporization rate model are numerically solved to predict aerodynamic droplet breakup in a high temperature gas environment. The numerical model accounts for variable properties and uses an adaptive local grid refinement technique on the gas-liquid interface to enhance the accuracy of the computations. The parameters examined include Weber (We) numbers in the range 15 – 90 and gas phase temperatures in the range 400 – 1000K for a volatile n-heptane droplet. Initially isothermal flow conditions are examined in order to assess the effect of Weber (We) and Reynolds (Re) number. The latter was altered by varying the gas phase properties in the aforementioned temperature range. It is verified that the We number is

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

Keywords: droplet breakup; VOF; heating; evaporation

1 Introduction

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

2 Numerical model and methodology

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

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

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

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

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

Table 1: Numerical settings used for the simulations.

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

3 Results and discussion

3.1 Cases examined and numerical setup

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

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

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

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

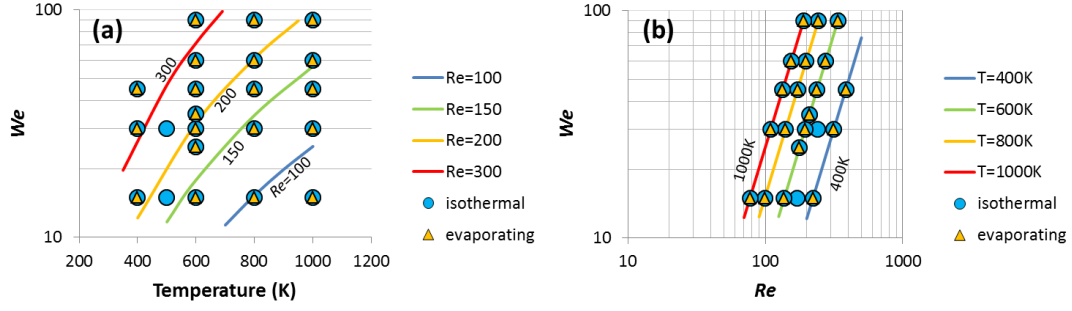


Fig. 1: Cases examined in (a) the $We-T_\infty$ plane and (b) the $We-Re$ plane.

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

3.2 Isothermal cases

3.2.1 General breakup behaviour

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

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

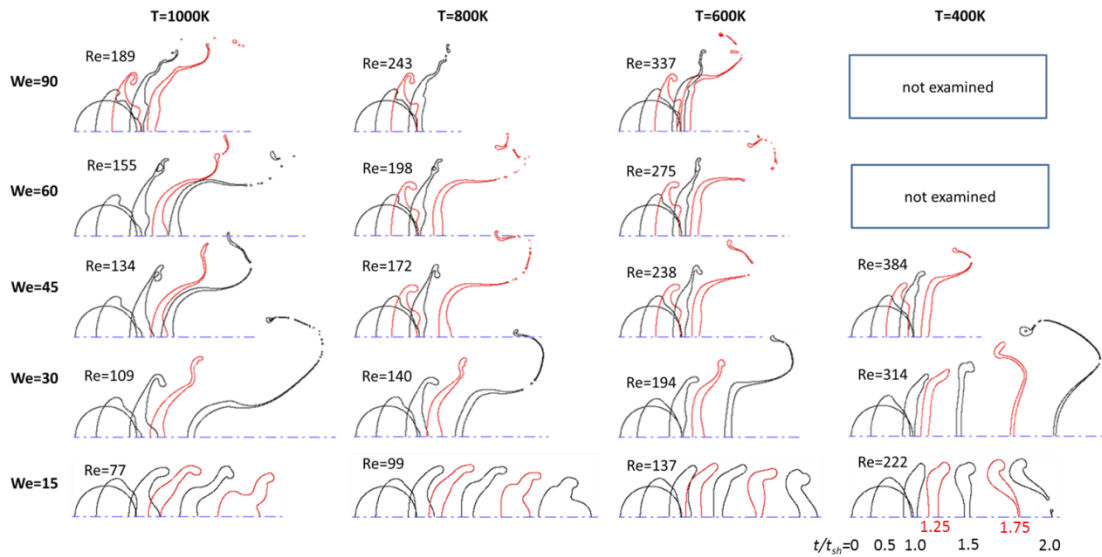


Fig. 2: Droplet shapes for the isothermal runs. The Re number increases from bottom to top and from left to right. The droplet shapes drawn black (see the online version) correspond to time

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

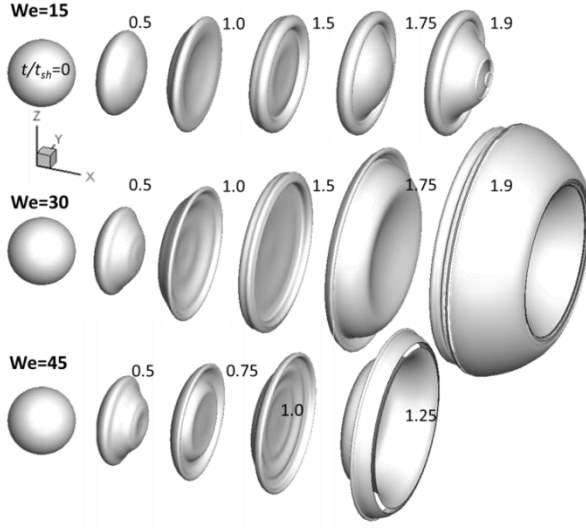


Fig. 3: Three-dimensional representation of the droplet shape evolution at three different We numbers examined for the isothermal cases corresponding to $T_{\infty}=400K$.

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

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

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

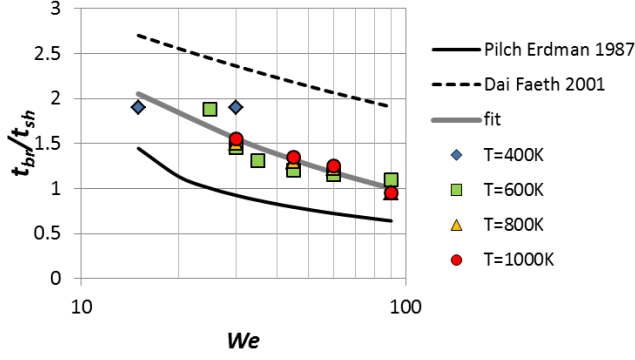


Fig. 4: Predicted dimensionless breakup time for the isothermal cases.

3.2.2 Measured quantities during breakup

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

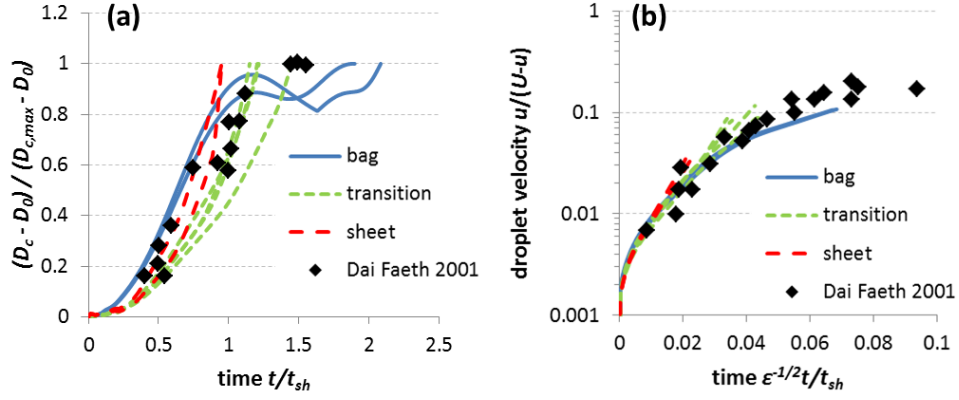
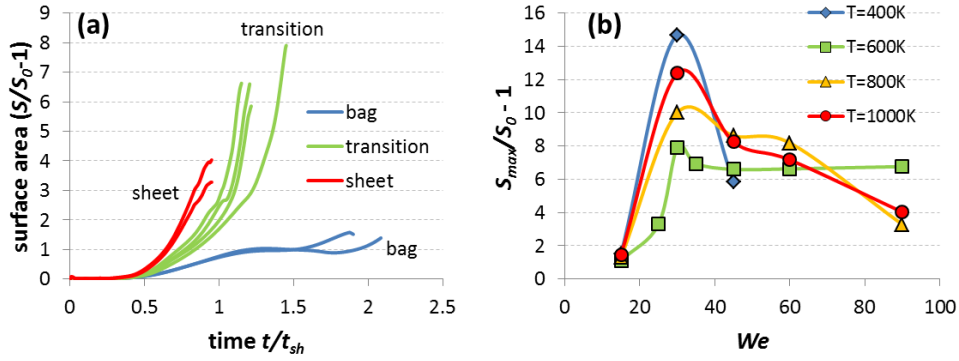


Fig. 5: Temporal evolution of (a) droplet's cross-stream diameter and (b) droplet's velocity for selected isothermal cases.

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

315



316

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

319

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

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

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

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

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

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

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

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

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

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

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

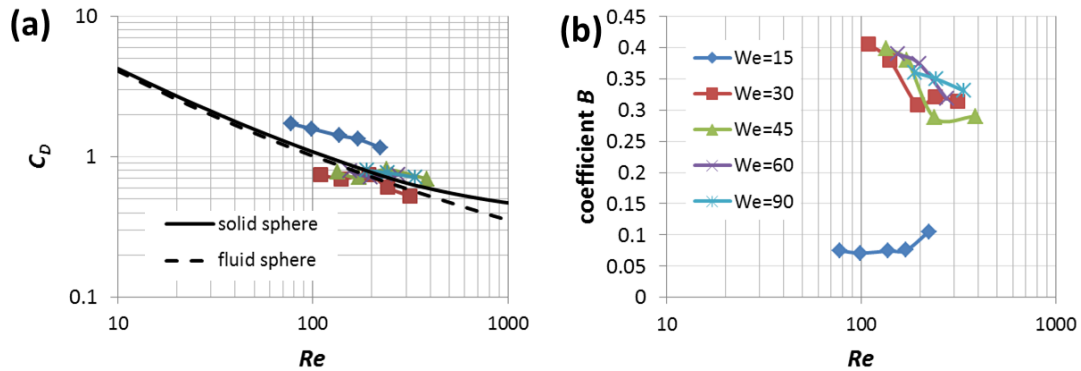


Fig. 7: (a) drag coefficient C_D and (b) coefficient B obtained from curve fitting of the droplet displacement data for the isothermal cases.

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

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

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

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

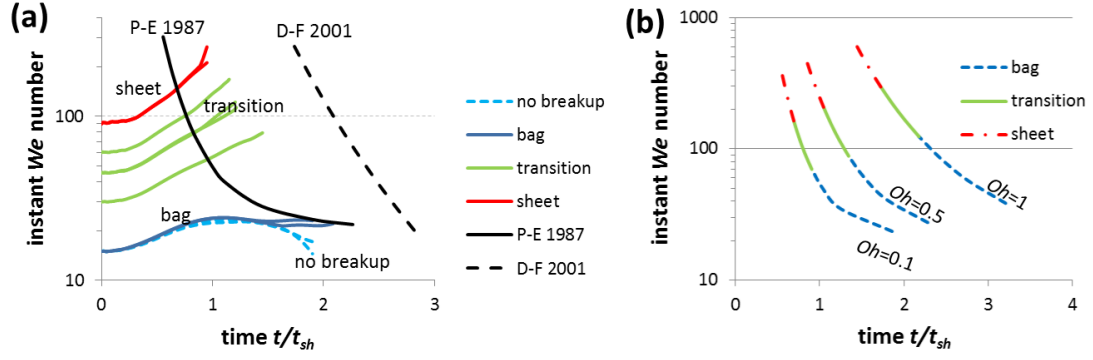
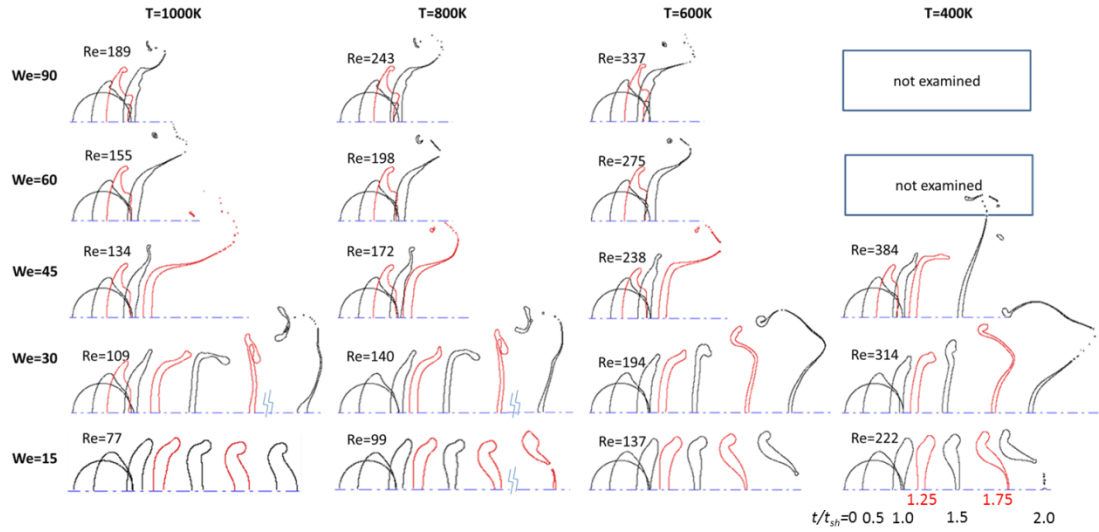


Fig. 8: (a) Predicted instant We number for selected isothermal cases and (b) instantaneous critical breakup conditions for various Oh numbers.

3.3 Evaporating cases

3.3.1 Hydrodynamic behaviour of the droplet

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



410

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

415

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

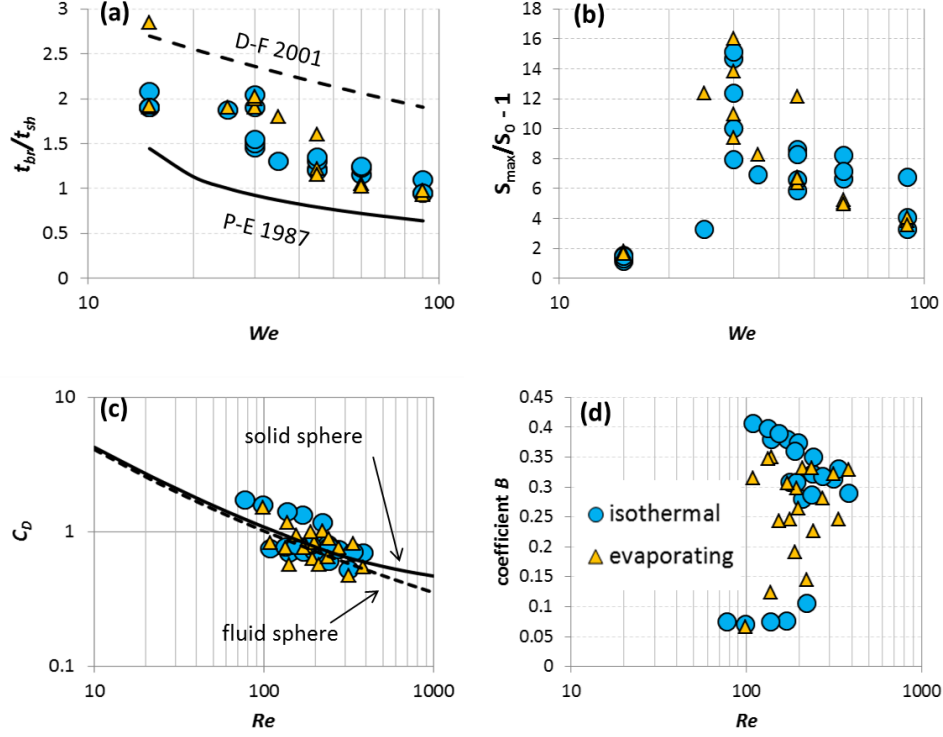


Fig. 10: Comparison of the predictions of the isothermal and the evaporating simulations for the (a) breakup instant, (b) maximum surface area, (c) drag coefficient and (d) coefficient B .

3.3.2 Thermal behaviour of the droplet

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

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

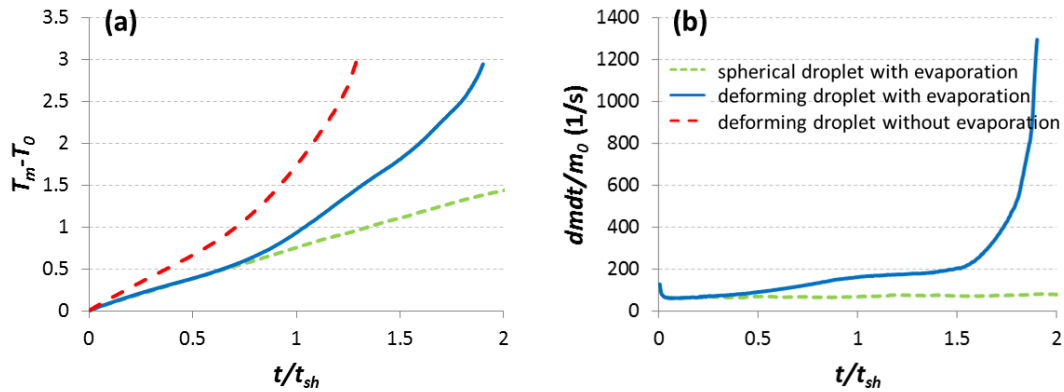


Fig. 11: Temporal evolution of (a) volume averaged droplet temperature and (b) evaporation rate for the case of $(We, T_\infty) = (30, 600)$.

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

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

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

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

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

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

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

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

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

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

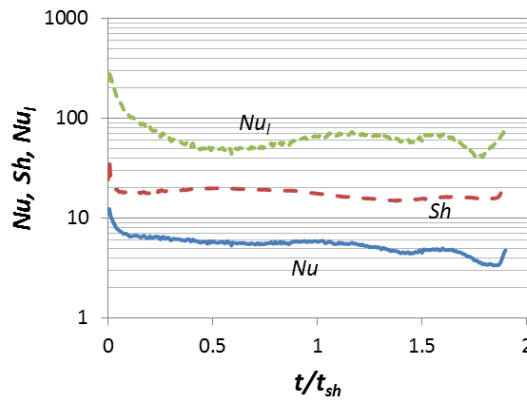


Fig. 12: Temporal variation of Nu , Sh and Nu_l for the case of $(We, T)=(30, 600)$.

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

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

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

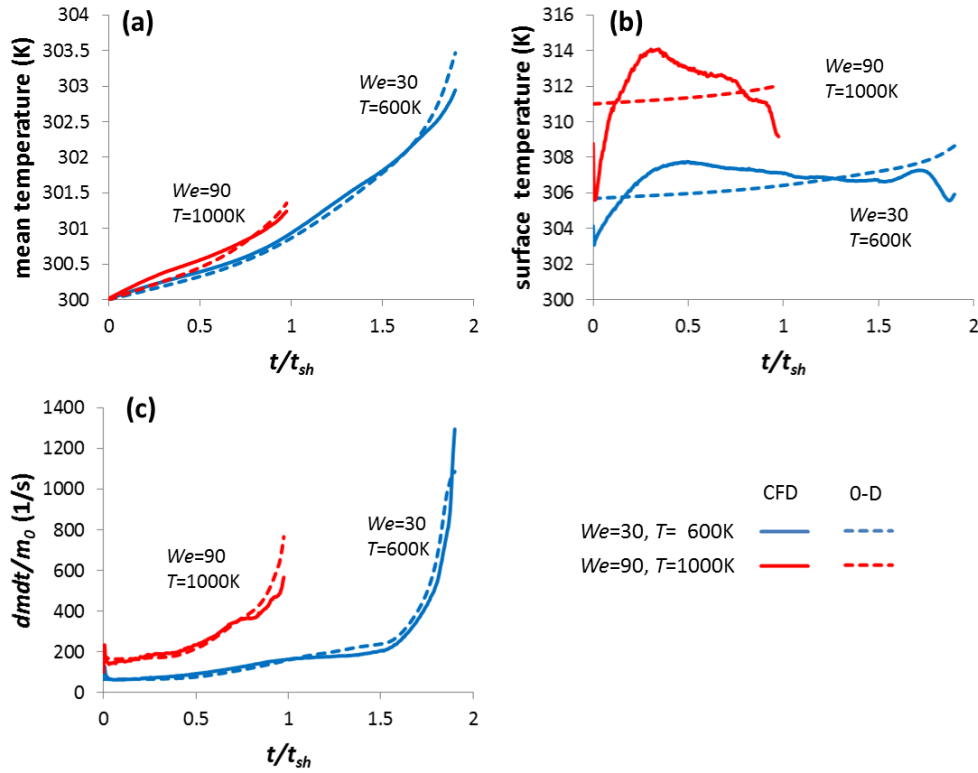


Fig. 13: Predictions of the 0-D model for (a) the volume averaged droplet temperature, (b) the surface temperature and (c) the evaporation rate. Solid lines are the CFD data and dashed lines are the 0-D model predictions.

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

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

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

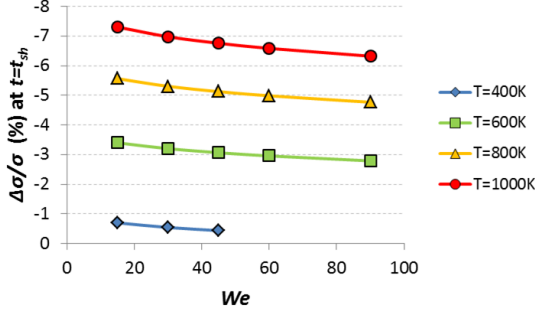


Fig. 14: 0-D model predictions for the percentage change of surface tension coefficient at $t=t_{sh}$ as a function of We number and gas phase temperature.

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

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

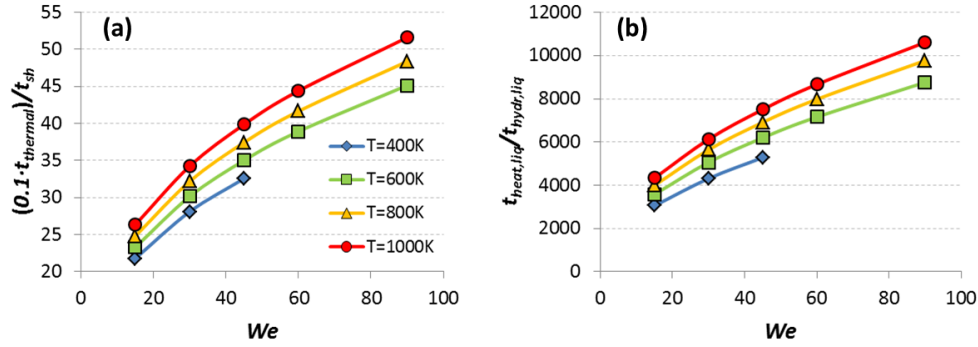


Fig. 15: Comparison of heating and flow timescales in (a) macroscopic and (b) microscopic level as a function of We number and gas phase temperature.

3.3.3 Spatial distribution of flow variables

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

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

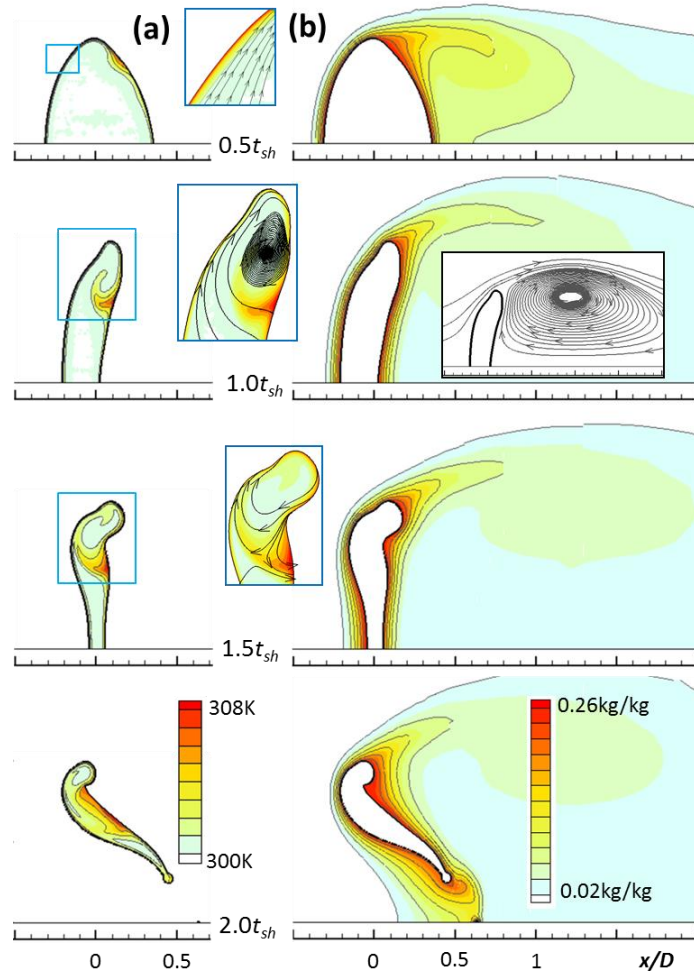


Fig. 16: Spatial distribution of (a) droplet temperature and (b) vapour concentration for the case
 $(We, T_\infty) = (15, 600)$. The inset figures aim to clarify the local relative velocity field.

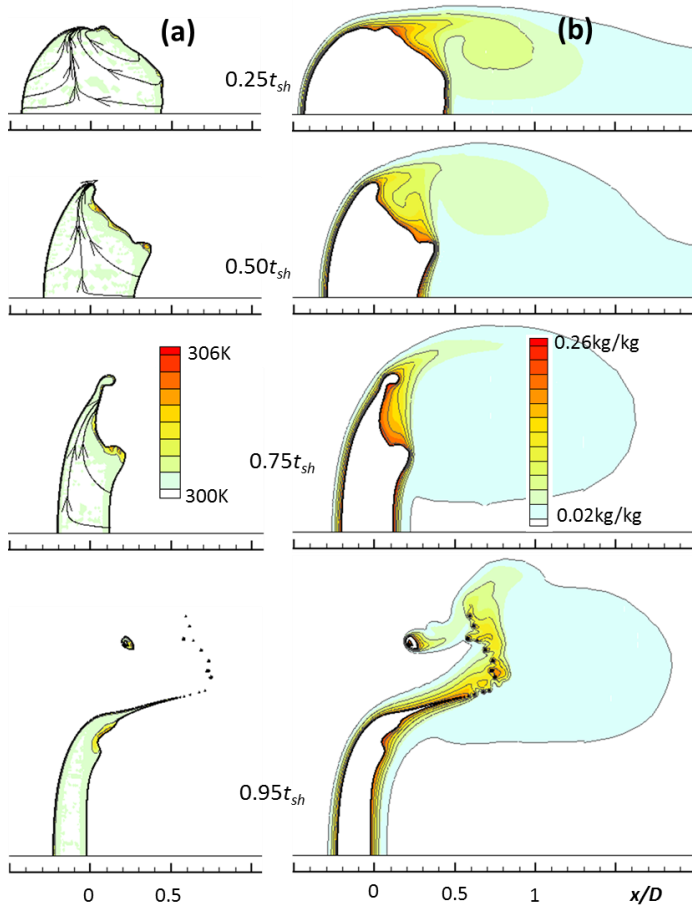


Fig. 17: Spatial distribution of (a) droplet temperature along with characteristic streamlines of the relative velocity field and (b) vapour concentration for the case $(We, T_\infty) = (90, 600)$.

4 Conclusions

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

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

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

5 Acknowledgements

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627 6 Nomenclature

628 Roman symbols

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

629

630

631 Greek symbols

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

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

632

Subscripts

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

633

Abbreviations

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

634

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636

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