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Full Length Article

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

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HIGHLIGHTS

- Drop breakup for various *We* and *Re* numbers at isothermal as well as evaporating conditions.
- VOF model coupled with a local evaporation model and adaptive grid refinement.
- Quantification of the effect of heating and evaporation on droplet breakup.
- Breakup is affected by heating mainly at low *We* numbers.
- An enhanced 0-D model is proposed to predict droplet heating and evaporation of deformed droplets.

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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 400–1000 K 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.

1. Introduction

Droplet breakup and evaporation are important physical processes controlling the efficiency of combustion systems; they are also realized 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

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Nomenclature

Roman symbols

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/kg K)
D	diameter (m)
D_{AB}	vapor diffusion coefficient (m^2/s)
Oh	Ohnesorge number $Oh = \mu_l/\sqrt{\rho_l \sigma D_0}$ (–)
k	thermal conductivity (W/m K)
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	vapor concentration (kg/kg)

Greek symbols

a	thermal diffusivity (m^2/s)
γ	thermal effusivity $\gamma = \sqrt{k\rho c_p}$ (J/m^2 K $s^{0.5}$)
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)

Subscripts

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

Abbreviations

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
VOF	volume of fluid

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:

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

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 and Ranger [9] is widely used:

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

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). Krzeczkowski [10] was one of first who presented a detailed breakup map in the We–Oh plane followed later by the studies of Hsiang and 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].