Direct Numerical Simulation of Droplet Deformation in External Flow at Various Reynolds and Weber Numbers

Anna Zotova, Yulia Troitskaya, Daniil Sergeev, and Alexander Kandaurov

Abstract Using the Basilisk software package, direct numerical simulation of the process of deformation of a liquid drop in a gas stream was carried out. The calculations were carried out for Reynolds numbers Re = 50–3000, Weber numbers We = 2–30. Two main modes of drop deformation were observed: bowl-shaped and dome-shaped, there is a transitional deformation mode between them. A map of deformation modes is constructed for comparison with the experimental data available in the literature. It was found that the dependence of the Weber number, corresponding to the transition from one deformation mode to another, on the Reynolds number is well described by the power law proposed in the literature.

Keywords Direct numerical simulation · Drop deformation mode

1 Introduction

The processes of deformation and secondary fragmentation of droplets play an important role in various industries: fuel, agriculture, etc. A lot of experimental work has been devoted to studying the behavior of a droplet in the flow of the external medium (Hsiang and Faeth, 1995; Krzeczkowski, 1980). Numerical experiments were also carried out to simulate the deformation and fragmentation of the droplet under the influence of a stationary external flow (Jalaal and Mehravaran, 2012; Kekesi et al., 2014; Pairetti et al., 2018). In the experiments, two types of perturbations leading to deformation and fragmentation of the droplet were investigated: a shock wave and steady disturbances. It was shown that the regime of droplet fragmentation under the influence of the shock wave depends on the ratio of the resistance forces of the medium and surface tension expressed by the Weber number $We = \rho_c d_0 u_0^2/\sigma$, and the ratio of the viscosity forces in the drop and the forces of surface tension expressed by the Ohnesorge number $Oh = \mu_d/(\rho_d d_0 \sigma)^{1/2}$, where d_0 and u_0 are the diameter

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of the droplet and its velocity relative to the medium velocity, ρ_c and ρ_d are the densities of the external medium and the droplet, respectively, μ_d is the viscosity of the droplet, and σ is the surface tension coefficient. As was shown in Hsiang and Faeth (1995), the mode of deformation and fragmentation of a droplet in a stationary flow is affected by the Weber number and Reynolds number $Re = \rho_c d_0 u_0/\mu_c$. The authors distinguish two types of droplet deformation in the external flow: dome-shaped and bowl-shaped. In the case of the dome-shaped deformation mode, the windward side of the droplet becomes flat, the leeward side remains rounded, this shape is similar to the shape of a droplet at the initial stage of the development of a bag-breakup phenomenon. For the bowl-shaped deformation mode, on the contrary, the leeward side of the drop becomes flat, and the conditions for the formation of bowl-shaped drops are to some extent similar to the conditions of shear-breakup and, apparently, are determined by the interaction between the drag and viscous forces. A map of the dome- and bowl-shaped modes of drop deformation obtained is presented in Fig. 2 of Hsiang and Faeth (1995). Based on a comparison of the shear stress with the surface tension forces, the authors propose the following estimate of the dependence of the Weber number corresponding to the transition from one mode to another on the Reynolds number: $We = 0.5 \cdot Re^{1/2}$.

2 Drop of Liquid in a Gas Stream

When conducting experimental studies, available equipment and materials usually impose a restriction on the set of problem parameters. So it seems relevant to conduct a numerical experiment that will remove this limitation. For direct numerical simulation of droplet deformation in the external flow, the Basilisk software package was used Popinet (2020). The Navier-Stokes equations for incompressible media with variable density are solved in Basilisk:

$$\rho\left(\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u}\right) = -\nabla p + \nabla \cdot (2\mu \mathbf{D}) + \sigma\kappa\delta_s \mathbf{n}, \tag{1}$$

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0, \tag{2}$$

$$\nabla \cdot \mathbf{u} = 0, \tag{3}$$

where $\mathbf{u}$ is the medium velocity, ρ is the density of the medium, μ is the dynamic viscosity and $\mathbf{D}$ is the deformation tensor defined as $D_{ij} \equiv \left(\partial_i u_j + \partial_j u_i\right)/2$. The surface tension term is concentrated at the interface, this is provided by the Dirac distribution function δ_s; σ is the surface tension coefficient, κ is the curvature, $\mathbf{n}$ is the normal to the interface.

Fig. 1 Configuration of the problem

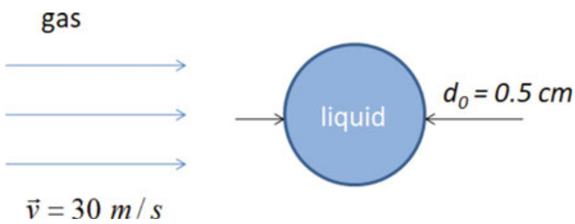

Table 1 Parameters used for modeling

d_0, m	u_0, m/s	ρ_d, kg/m^3	ρ_c, kg/m^3	μ_d, Pa·s	μ_c, Pa·s	σ, N/m
0.005	30	1000	1.2	1.003e-3	$\rho_c d_0 u_0 / Re$	$\rho_c d_0 u_0^2 / We$

For two-phase flows the volume fraction c of the first liquid is introduced, and the density and viscosity are determined as

$$\rho \equiv c\rho_1 + (1 - c)\,\rho_2, \tag{4}$$

$$\mu \equiv c\mu_1 + (1 - c)\,\mu_2, \tag{5}$$

where ρ_1, ρ_2 and μ_1, μ_2 are the densities and viscosities of the first and second media, respectively.

We examined the problem of the following geometry: a drop of liquid with a diameter 5 mm was placed in a gas stream at a speed of 30 m/s (see Fig. 1). The density of the liquid ρ_d and gas ρ_c correspond to the density of water and air, the viscosity of the liquid μ_d is equal to the viscosity of water. The viscosity of the gas μ_c and the surface tension at the interface between the liquid and gas σ are determined by the set values of the Reynolds and Weber numbers (see Table 1).

When considering the deformation and fragmentation of a liquid drop in a gas stream, the characteristic shear fragmentation time proposed in Ranger and Nicholls (1969) is introduced:

$$t^* = d_0\,(\rho_d/\rho_c)^{1/2}\,/u_0 \tag{6}$$

According to measurements made by Cao et al. (2007); Dai and Faeth (2001), the initial deformation of a drop occurs in a dimensionless time approximately equal to $t/t^* = 1 - 2$ and weakly depends on the Weber number (in the range considered by the authors, see Cao et al. (2007) Fig. 7). For the parameters under consideration $t^* = 5.3$ ms, in our work we considered the deformation of the droplet at time $t = 5.5$ ms.

3 Results

In order to observe the transition from bowl-shaped to dome-shaped deformation of the droplet, a simulation was performed with parameters corresponding to Weber numbers We = 2–30 and Reynolds numbers Re = 50–3000.

The process of droplet deformation for the bowl-shaped (Re = 50, We = 12) and dome-shaped (Re = 1000, We = 6) modes is shown in the Fig. 2. It can be noted that for these parameters of the bowl-shaped mode, the shape of the drop changes significantly over time, for example, after 3 ms the drop has a narrow ledge in the direction of the wind.

Figure 3 shows an example of the obtained simulation results - a droplet shape 5.5 ms after placing a spherical droplet in a gas stream for Weber numbers We = 8 and We = 12 and various Reynolds numbers. It can be seen that for the Weber number We = 12, the bowl-shaped mode of deformation of the drop occurs at Reynolds numbers Re = 50–300, the dome-shaped mode—at Re = 500–1000. The transition from one mode to another occurs when the Reynolds number is about Re = 400. For the Weber number We = 8, the transition from one mode to another is shifted to the range of Reynolds numbers Re = 200–300.

A map of the dome- and bowl-shaped modes of drop deformation for different Weber and Reynolds numbers is shown in Fig. 4. The results corresponding to the bowl-shaped mode of deformation of the droplet are shown by black squares, and the dome-shaped mode by red circles. Transitional mode is marked by green stars.

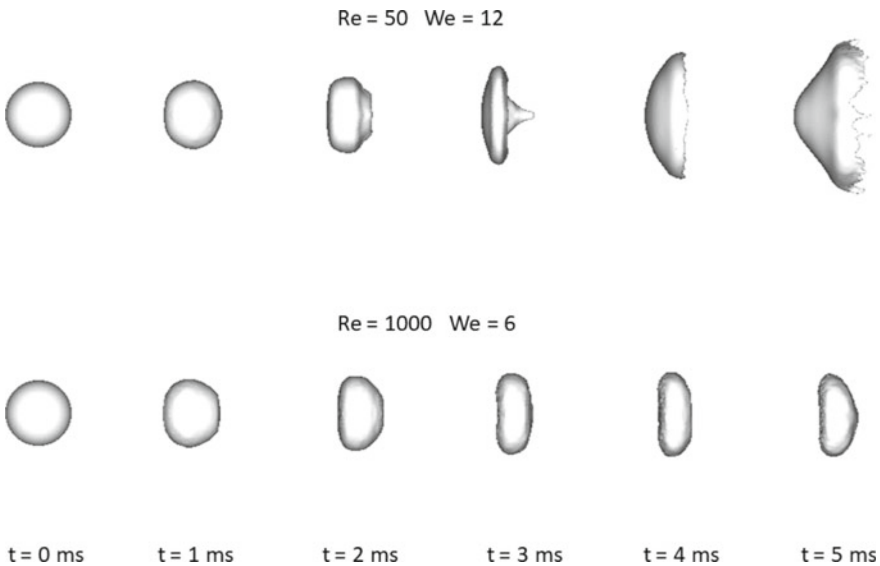

Fig. 2 Drop deformation for different points in time: bowl-shaped (Re = 50, We = 12) and dome-shaped (Re = 1000, We = 6) modes

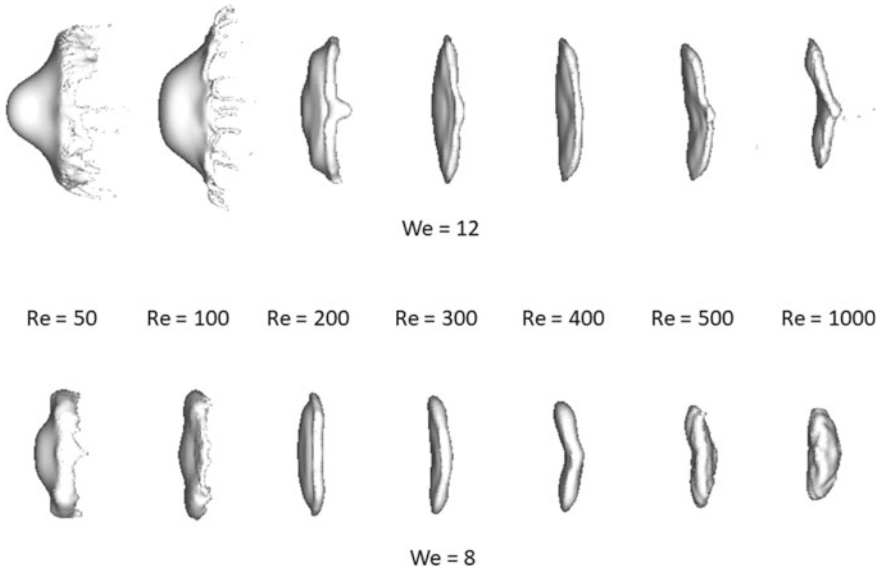

Fig. 3 The result of numerical simulation of droplet deformation in a gas stream with parameters corresponding to the Weber numbers We = 12 and We = 8 and various Reynolds numbers Re at time t = 5.5 ms.

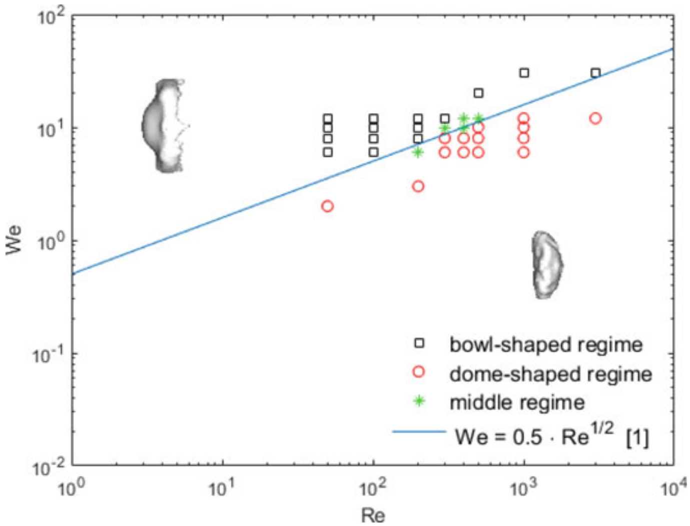

Fig. 4 Map of dome-shaped and bowl-shaped modes of drop deformation obtained as a result of numerical experiments. The line shows the dependence of the Weber number corresponding to the transition from one regime to another, on the Reynolds number obtained in Hsiang and Faeth (1995)

The blue line corresponds to the dependence of the Weber number corresponding to the transition from one regime to another on the Reynolds number proposed in Hsiang and Faeth (1995): $We = 0.5 \cdot Re^{1/2}$ (see Fig. 2 of the work Hsiang and Faeth (1995)). It can be seen that the results obtained using direct numerical simulation are in agreement both with this dependence and with the experimental data obtained in Hsiang and Faeth (1995).

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