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Detailed numerical simulation of unsteady drag coefficient of deformable droplet

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Unsteady drag coefficient is larger than steady drag coefficient for decelerating relative flow.

The unsteady term has the most effect on the unsteady drag coefficient.

Linear correlation between drag coefficient difference and unsteady parameter is obtained for low Weber number.

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The detailed numerical simulation of the unsteady drag coefficient of deformable droplet is investigated with a mass conserving level set (LS) method. The simulation results indicate that the unsteady drag coefficient is always larger than the steady standard drag coefficient for the present decelerating relative flow. The effects of Weber number, density ratio and viscosity ratio on the unsteady drag coefficient of drop deformation are studied. It is found that the unsteady term (including density ratio) has the most effect on the unsteady drag coefficient and Weber number secondly. The viscosity ratio has little effect on the unsteady drag coefficient due to low Ohnesorge number. The numerical results confirm that the difference between drag coefficient and standard steady drag coefficient has an approximately linear curve fit with the unsteady parameter for low Weber number. These results will lay the foundation for the modeling of unsteady drag coefficient in our further work.

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1. Introduction

Liquid atomization is a common phenomenon in a variety of scientific and engineering applications, such as mixing, spraying, printing, food processing, agriculture, pharmaceutical process and combustion devices in gas turbine. The atomization process is complex, involving highly turbulent and convoluted interfaces as well as breakup and coalescence of liquid masses [\[1\].](#page--1-0) The atomization process of liquid can be divided into two consecutive steps, the primary and the secondary atomization. The initial breakup of the liquid bulk into filaments and structures is called the primary atomization, whereas the subsequent breakup of these filaments and structures into smaller droplets is called the secondary atomization.

Since the secondary atomization has a significant effect on the final drop size distribution (DSD) which is the goal of many atomization processes, it is important to determine the move-

⇑ Corresponding author. E-mail address: zjulk@zju.edu.cn (K. Luo). ments of these small droplets. The behaviors of drops embedded in the gas phase have been investigated for many years. The well-known Stokes equation, standard drag coefficient curve of steady drop and Oseen's solution are reviewed in widely accessible literatures [\[2\].](#page--1-0) In multiphase flows, the droplets are different from the solid particles due to deformation and internal circulations in the droplets. Hence, the modeling of the behaviors of droplets should be different from the formulation that is applied to solid particles.

For the experiments, there are some studies on drag force of droplets [\[3–6\].](#page--1-0) However, the physical processes at the interface of two phases often occur at small time and length scales that experimental apparatus are not capable of fully observing them. Moreover, owing to lack of access to velocity and pressure fields, the results of experiments are mainly limited to qualitative results, such as breakup modes. For the theoretical studies, a lot of assumptions and approximations are necessary and it is ineffective in representing the present complexity and chaotic unsteady movement of droplet. To date numerical simulation has become a common practice and probably the best way to gain insight into

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the details of small scale physics in interfacial multiphase flows [\[1\].](#page--1-0) As mentioned by Guildenbecher et al. [\[7\],](#page--1-0) direct numerical simulation (DNS) of Navier-Stokes equations combined with interface tracking is the best known technique for the representation of gas–liquid interface. Therefore, the present work is conducted using DNS to investigate the drag coefficient that is important to the modeling of movement of droplet.

There have been some numerical studies reported in the literatures where the focus is on the breakup of drops rather than the drag coefficient. By using a finite difference/front tracking technique, Han and Tryggvason [\[8\]](#page--1-0) simulated the secondary breakup of liquid drop accelerated by a constant body force at low density ratio of 1.15 and 10. Moreover, Han and Tryggvason [\[9\]](#page--1-0) also conducted the simulation of liquid drop breakup by an impulsive acceleration at the same density ratio in $[8]$. Khosla et al. $[10]$ used the volume-of-fluid (VOF) method to provide insights into the breakup of a liquid drop by gas crossflow and found that the liquid drop follows the surface wave driven, sheet breakup mechanism, which is contrary to the boundary layer stripping theory. By using the level set (LS) method to capture the liquid/gas interface, Liu and Xu [\[11\]](#page--1-0) obtained four typical breakup modes and found the gas Weber number was of the highest importance. Other references related to the drop breakup can be found in [\[12–19\]](#page--1-0).

Nevertheless, there are a limited number of studies which investigate the drag coefficient of deformable drops. Deformation and drag coefficients of decelerating drops were numerically computed by Wadhwa et al. $[20]$ and the drag coefficients are compared with those of solid spheres. The dependence on the gas-based Weber number and the Ohnesorge number are also discussed. Feng [\[21\]](#page--1-0) performed the simulation of a deformable liquid drop falling through a quiescent gas at large density ratio of 1000 and viscosity ratio from 50 to 1000. The effects of Reynolds number, Weber number and viscosity ratio on the morphology were investigated and it was shown that the drag coefficient agreed well with an empirical formula using the cross-sectional area. Khare and Yang [\[22\]](#page--1-0) investigated drag coefficients of deforming and fragmenting liquid droplets over a broad range of Reynolds numbers $(10^3 < Re < 10^5)$ and Weber numbers $(20 < We < 1400)$. Their results showed that the drag coefficient increased to a maximum as the droplet frontal area increased and then decreased at the initiation of breakup. It was also found that the averaged drag coefficients decreased with increasing Weber number as a power law. Quan and Schmidt [\[23\]](#page--1-0) studied the drag force and the deformation of a liquid droplet impulsively accelerated by gaseous flow using a moving mesh interface tracking approach. It was found that the total drag coefficients are larger than typical steady-state drag coefficients of solid spheres at the same Reynolds numbers, which agrees with the experimental results. The Reynolds numbers were restricted to 10 < Re < 40. The initial Weber number and the viscosity ratio were demonstrated to have significant effects on the droplet dynamics.

However, three dimensional simulations of drag coefficient of deformable drops are still limited to now due to the challenges of representing time-dependent deformable interfaces. For the modeling purpose, the drag coefficient, especially the unsteady effect, is crucial but is investigated in limited references. Therefore, it is imperative to study the unsteady drag coefficient and the effects of factors on it. In addition, the effects of droplet deformation (Weber number controlled) and internal circulation (viscosity ratio controlled), which is different from the solid sphere particles, are still unknown.

The aim of the work presented in this paper is to study unsteady drag coefficient of liquid droplet by using a conserving LS method. The outline of the present study is organized as follows. In Section 2, we provide the governing equations and describe the LS method. In Section [3,](#page--1-0) we present numerical configurations and computational cases. In Section [4](#page--1-0), we discuss the time history of the unsteady drag coefficient evolution and the effects of Weber number, density ratio and viscosity ratio on the unsteady drag coefficient.

2. Numerical methods

2.1. Governing equations

The Navier-Stokes equations for gas and liquid phases read

$$
\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho} \nabla p + \frac{1}{\rho} \nabla \cdot (\mu [\nabla \mathbf{u} + \nabla \mathbf{u}^t]),\tag{1}
$$

$$
\frac{\partial \rho}{\partial t} + \mathbf{u} \cdot \nabla \rho = 0, \tag{2}
$$

where **u** is the velocity, ρ is the density, p is the pressure and μ is the dynamic viscosity. The material properties of gas and liquid are constant, i.e., $\rho = \rho_l$, $\mu = \mu_l$ in liquid phase and $\rho = \rho_g$, $\mu = \mu_g$ in gas phase and they are subjected to jump conditions at the interface, namely, $[\rho]_{\Gamma} = \rho_l - \rho_g$ and $[\mu]_{\Gamma} = \mu_l - \mu_g$. The velocity across the interface is continuous, i.e., $[\boldsymbol{u}]_{\Gamma} = 0$. The pressure across the interface can be expressed as

$$
[p]_{\Gamma} = \sigma \kappa + 2[\mu]_{\Gamma} \mathbf{n}^t \cdot \nabla \mathbf{u} \cdot \mathbf{n},\tag{3}
$$

where σ is the surface tension, κ is the interface curvature and **n** is the interface normal.

The discretization of the Navier-Stokes equations is based on the staggered uniform grid, in which the pressure p and the LS function G are stored at the cell centers, while velocity is stored at the face centers. The spatial discretization of the Navier-Stokes equations is performed using the second-order finite central difference schemes. The second-order semi-implicit iterative procedure [\[24\]](#page--1-0) for time integration is utilized, which is efficient, stable and accurate. The iteration can be expressed as

$$
u_{k+1}^{n+1} = u^n + \Delta t f \left[\frac{1}{2} \left(u^n + u_k^{n+1} \right) \right] + \frac{1}{2} \Delta t \left[\frac{\partial f}{\partial u} \right] \left(u_{k+1}^{n+1} - u_k^{n+1} \right) \tag{4}
$$

where f is the right hand side of Navier-Stokes equations, and $\partial f / \partial u$ is the Jacobian. The computations of velocity and pressure fields are decoupled by using the projection method.

2.2. Interface capturing method

The LS method is used to capture the interface, which is implicitly given by the zero iso-surface of the smooth LS function $\phi(\mathbf{x},t)$. Generally, the LS function ϕ is imposed to be the signed distance function to the interface, i.e.,

$$
|\phi(\mathbf{x},t)| = |\mathbf{x} - \mathbf{x}_{\Gamma}| \tag{5}
$$

where x_{Γ} is the location at the interface that is closest to x. The LS function is defined to be positive for the liquid phase and negative for the gas phase.

However, the LS method suffers the issue of mass loss. Instead of using the signed distance function, the hyperbolic tangent function ψ proposed by Olsson and Kreiss [\[25–26\]](#page--1-0) is employed here,

$$
\psi(\mathbf{x},t) = \frac{1}{2} \left(\tanh \left(\frac{\phi(\mathbf{x},t)}{2\varepsilon} \right) + 1 \right)
$$
(6)

where ε is the thickness of the profile. The evolution of the interface is implicitly captured by the LS equation,

$$
\frac{\partial \psi}{\partial t} + \nabla \cdot (\mathbf{u}\psi) = 0 \tag{7}
$$

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