Direct Numerical Study of a Liquid Droplet Impulsively Accelerated by Gaseous Flow

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Abstract
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Direct numerical study of a liquid droplet impulsively accelerated by gaseous flow

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A liquid spherical droplet impulsively accelerated by a gaseous flow is simulated in order to investigate the drag force and the deformation. The dynamics of the droplet immersed in a gaseous flow are investigated by solving the incompressible Navier-Stokes equations using a finite volume staggered mesh method coupled with a moving mesh interface tracking scheme. The benefit of the current scheme is that the interface conditions are implemented directly on an explicitly located interface with zero thickness. The droplet shape changes as it is accelerated, and the deformation factor of the droplet is as small as 0.2, so mesh adaptation methods are employed to achieve good mesh quality and to capture the interface curvature. The total drag coefficients are found to be larger than typical steady-state drag coefficients of solid spheres at the same Reynolds numbers. This agrees with the observation of Temkin et al. [J. Fluid Mech. 96, 133 (1980)] that the unsteady drag of decelerating relative flows was always larger than the steady drag. The large recirculation region behind the deformed droplet may explain this greater drag force. The effects of the viscosity ratio, density ratio, and initial Weber number on the droplet dynamics are also studied. It is found that the initial Weber number and the viscosity ratio have significant effects on the droplet dynamics, while the density ratio does not. © 2006 American Institute of Physics. [DOI: 10.1063/1.2363216]

INTRODUCTION

The dynamics of droplets in a gaseous flow are of great interest for engineers and scientists from a large variety of disciplines. Rainfall, sprays, and ink jet printing are only a few of the phenomena and processes in which droplets play primary roles. The most fundamental coupling of the gas and liquid phases comes from drag forces. In multiphase flow simulations using reduced models for droplet behavior, drag must be calculated correctly in order for the calculations to have any predictive value. Such drag models are difficult to formulate, because momentum transfer between the droplet and the ambient gas may result in large acceleration and deformation, even in the absence of breakup. These interactions, despite being fundamental, are still not well understood as they happen on tiny length scales and very short time scales. It is well known that spherical droplets undergo significant deformation and acceleration, and then become flattened due to the drag forces from the surrounding gas. Deformation increases the drag forces due to both the larger frontal area and an increase of the drag coefficient ($C_D$). However, in many multidimensional spray simulations, the drag correlations for spheres in steady flows are used to estimate the momentum exchange between the droplets and the surrounding gas. A low Weber number is typically used to justify this simplification.

Though consideration of internal circulation is quite common, the effects of deformation have proven more difficult to quantify. Steady-state investigations have measured the difference between the steady drag coefficients for solid spheres and spheroids.6-7 Hsiang and Faeth8 performed experimental measurements of droplets subjected to shock waves with high Reynolds numbers and large density ratios, and they found that the drag coefficient was a function of the deformation. Helenbrook et al.9 numerically studied the dynamics of quasisteady liquid drops, and they noted the quasisteady drag of a liquid drop was different from that of a solid sphere.

The transient nature of droplet deformation creates an additional parameter that can affect drag; transient drag may depend on Ohnesorge number and history forces. Recently, Wadhwa et al.10 numerically simulated transient drop-gas flows by a hybrid compressible-incompressible method in order to study a decelerating liquid droplet. Han et al.11 and Aalburg et al.12 numerically investigated axisymmetric liquid drops that were accelerated impulsively, where the density differences between the drops and the ambient fluid were small. Temkin et al.13,14 experimentally studied droplet drag in accelerating and decelerating flows. The Weber numbers of the droplets were very small, so the deformation of the droplets was tiny. They showed that, for flows with decreasing relative velocities, the unsteady drags were always larger than the steady values at the same Reynolds numbers, while the unsteady drags were always smaller than the steady values for accelerating relative flows.

This paper presents the numerical simulations of a liquid
droplet accelerated impulsively by gas flow. To address this challenge, a three-dimensional finite volume staggered mesh method coupled with a moving mesh interface tracking scheme is employed, combined with adaptive mesh methods that are used to achieve good mesh quality and to deal with large deformation. The Reynolds numbers of the simulations are in the range of Temkin et al.’s, and the numerical results are compared with their observations. Larger values of Weber number, above what Temkin et al. studies, will be simulated in order to better understand the role of droplet deformation. The effects of the density ratio, the viscosity ratio, and the surface tension on the droplet dynamics are also presented in this paper.

**FORMULATION AND NUMERICAL METHOD**

**Governing equations and problem setup**

The physical problem and computational domain are sketched in Fig. 1. Initially, the droplet is located in the middle of a box domain. The droplet has an initial radius \( r_0 \), and the box has a length of \( 48r_0 \), width of \( 16r_0 \), and height of \( 16r_0 \). The box domain is large enough so that the boundary effects can be assumed small. The upper and lower walls are moving walls with the same velocity, and the two sides are slip walls. An inlet boundary condition with uniform velocity is enforced on the left side of the domain and an outlet boundary on the right side. The immiscible, incompressible two-phase flow is solved by a finite volume method with a moving mesh, and the governing equations are (see Ref. 15)

\[
\frac{d}{dt} \int \int \int_{CV} \rho u dv + \int \int_{CS} \rho u \cdot n ds = 0,
\]

\[
\frac{d}{dt} \int \int \int_{CV} \rho dv + \int \int_{CS} \rho (u - v) \cdot n ds = 0,
\]

where \( CV \) is a control volume, \( CS \) stands for the surface of the control volume, \( u \) is the fluid velocity, \( v \) is the surface velocity of the control volume, \( n \) stands for the unit vector of the face normal, \( f \) denotes the body force per unit mass, and the superscript \( T \) stands for the transpose. Equation (1) is the conservation of volume, which indicates that the rate of volume change is equal to a closed control surface integral of \( v \). This equation is a consistency requirement that can be derived from Leibnitz’s theorem.

The boundary conditions across the interface are

\[
u_{1n} = u_{2n} = v_n,
\]

\[
[u] = 0,
\]

\[
[p] = -\sigma \left( \frac{1}{R_1} + \frac{1}{R_2} \right) + 2\mu (\nabla u \cdot n) \cdot n,
\]

\[
\left[ \mu \left( \frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) n_j \right] = 0,
\]

where \( \sigma \) stands for the surface tension coefficient and is assumed to be a constant, \( R_1 \) and \( R_2 \) are the principal radii of the surface, \( \tau \) denotes the tangential unit vector, and \([ \ ]\) stands for the difference across the interface.

The numerical scheme solves an exact projection formulation of the governing equations using a finite volume staggered mesh method.\(^{15,17}\) The surface tension force is evaluated by a least-squares parabola fitting method,\(^{18}\) and the interface is moved in a Lagrangian mode to conserve mass. The Lagrangian motion of the interface naturally follows the characteristics of convection, for a high-fidelity rendering of the surface,\(^{21–23}\) used an adaptive restructuring of surface mesh method to compute drop breakup and coalescence, and also presented an adaptive unstructured volume remeshing scheme coupled with a level set method to simulate multiphase flow. However, in the present work, the additional constraint of maintaining the interface shape and fluid identity was imposed on flipping. The approach to mesh smoothing also differs. Cristini and co-workers\(^{21–23}\) used a spring-analogy approach for solving for node motion. The present work uses an optimization process described in prior publications.\(^{19,20}\)

The boundary conditions across the interface are implemented explicitly in the two-phase flow solver, and the geo-

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**FIG. 1.** Sketch of a droplet in a moving gaseous flow.
metric harmonic mean method is used for calculating the interface shear stress.\textsuperscript{20} A three-step, second order, low storage, Runge-Kutta scheme is used for time advancement. The details of the three-step scheme can be found in Ref.\textsuperscript{15}.

Careful construction of the initial condition is required, in order to represent the impulsive acceleration by a gas stream. The initial condition must be divergence-free with a smooth velocity field. Because the gas is incompressible, the passage of a shock wave cannot be represented. Instead, the liquid initial velocity was set to zero and the steady-state velocity field of the gas phase was calculated. First, a uniform velocity field is assumed for the gas, creating large momentum errors at the interface, which is shown in Fig. 2(a). Obviously, the simulation cannot continue with these discontinuous velocity distributions. The simulation is run with the mesh fixed, and by treating the droplet as a solid for some time, the velocity jump will be smoothed out by the viscous, producing a continuous velocity field at the interface. The smoothed flow fields are shown in Fig. 2(b), and these flow fields are then taken as the initial condition for the simulation.

![FIG. 2. Velocity distributions in a $yz$ plane slice. The velocity vectors are colored by magnitude. (a) Initial velocities for the droplet accelerated by gaseous flow. The black lines denote the outer boundaries. The droplet is in black. (b) Smoothed velocities for the droplet accelerated by gaseous flow. The droplet is in gray.](image)

![FIG. 3. Two-dimensional sketch of a droplet in a moving gaseous flow.](image)
droplet impulsively accelerated by a gaseous flow. Note that
the recirculation region behind this spherical droplet is very
small.

Definition of deformation factor and drag coefficient

The deformation factor $D$ of the droplet is defined as

$$D = \frac{a}{b},$$

where $a$ is the length of the shortest axis and $b$ is the length of
the longest axis. The configuration of the case is shown in Fig. 3.

The Reynolds number and Weber number are defined based on
the relative velocity and the gas properties as

$$Re_g = \frac{\rho_g (U_g - U_c) 2 r_0}{\mu_g}, \quad We_g = \frac{\rho_g (U_g - U_c) 2 r_0}{\sigma},$$

where $U_g$ is the free stream gas velocity, $U_c$ stands for the
droplet centeroid velocity, $\rho_g$ denotes the gas density, $r_0$ is
the sphere droplet radius, and $\mu_g$ denotes the gas-phase dy-
namic viscosity. The droplet centroid velocity ($U_c$) is calcu-
lated by taking the volume average of the cell velocities in-
side the droplet. The initial Reynolds number and the initial
Weber number are

$$Re_{g,i} = \frac{\rho_g U_g 2 r_0}{\mu_g}, \quad We_{g,i} = \frac{\rho_g U_g^2 2 r_0}{\sigma},$$

respectively. The subscript $i$ indicates that these are the initial
values of Reynolds and Weber numbers. Similar to Temkin
and Kim, the equation for the droplet acceleration is
where \( C_D \) is the total drag coefficient, which includes added mass, history effects, and other forces. The full Basset-Boussinesq-Oseen equation cannot be applied directly in this case, since there is no closed-form solution for the general case of a deforming droplet. In the definition of drag coefficient used here, the initial droplet radius is used in calculating frontal area, since the droplet deformation is not known \emph{a priori}. As a consequence of this definition, the coefficient of drag represents several combined effects.

Then the total drag coefficient can be calculated from acceleration by

\[
\frac{4}{3} \pi r_0^3 \frac{dU_c}{dt} = \frac{1}{2} \rho_g \pi r_0^2 (U_g - U_c)^2 C_D,
\]

\[
C_D = \frac{8}{3} r_0 \eta \frac{dU_c}{dt} \left( \frac{U_g - U_c}{U_g - U_c} \right)^2,
\]

where \( \eta = \rho_d / \rho_g \) is the density ratio, and the viscosity ratio is defined as \( \lambda = \mu_d / \mu_g \).

**RESULTS AND DISCUSSION**

The numerical method for three-dimensional two-phase flows was validated against analytical and experimental results, and it was found that the method is accurate and robust in solving multiphase flows. In this section, the simulation for a droplet impulsively accelerated by a gas flow with
Re_{e,j}=40, \text{ We}_{e,j}=40, \text{ and } \lambda = \eta = 50 \text{ is presented. The effects of the initial Weber number, the density ratio, and viscosity ratio on droplet dynamics are also studied. Finally, the mesh dependence of the numerical method is evaluated by using two different mesh resolutions. Because two-phase flow simulations traditionally demonstrate very poor convergence characteristics,\textsuperscript{24} demonstrating mesh independence is essential for establishing confidence in the results.}

**Numerical results for the case with Re_{e,j}=40, \text{ We}_{e,j}=40, \text{ and } \lambda = \eta = 50**

In Fig. 4, the deformation of the droplet at different times is shown for Re_{e,j}=40, \text{ We}_{e,j}=40, \text{ and } \lambda = \eta = 50. It can be seen clearly that the droplet is deforming, and at t=15.0, the initial sphere droplet becomes flattened, where t is non-dimensionalized by \(U_i/r_0\). The mesh adaptations make the mesh finer at the edge of the droplet to capture the curvature as well as droplet dynamics. The deformation history of the droplet is illustrated in Fig. 5(a), and the deformation factor is as small as 0.2. The droplet deforms faster in the early stage, but slower in the later time. This is because as the droplet deforms, the surface tension plays a more significant role due to the larger curvature at the edge of the droplet. The relative velocity decreases as the droplet accelerates, and this leads to the decreasing of Re_g with time as shown in Fig. 5(b). Figure 5(c) gives the drag coefficient versus Reynolds number, and it indicates that the drag coefficient is increasing as the Reynolds number decreases. Comparing the numerical results with Temkin et al.‘s\textsuperscript{13,14} experimental observations (as shown in Fig. 6), the simulation predicts comparable drag coefficients to the experimental measurements when the Weber numbers matched. Both the predicted and experimental measurements were much larger than the standard \(C_D\). Here, the standard \(C_D\) stands for the drag coefficient determined experimentally using techniques that lead to steady measurements, and it is applicable only to rigid spheres moving steadily in a fluid. This means that the standard drag coefficient includes neither history effects nor the deformation of the droplet. The details of the definition of the standard \(C_D\) can be found in Temkin et al.’s paper.\textsuperscript{13}

Once the predictions had been validated using Temkin et al.’s results, the effects of Weber number were explored. The Weber numbers of Temkin et al.’s experiments varied only from 0.001 to 4.0. In order to better understand the effect of surface tension and droplet distortion, high Weber numbers, above the range investigated by Temkin et al., were simulated. These high Weber number simulations produced more drag coefficients than Temkin et al.’s data due to the large predicted droplet distortion.

The simulation results further confirm Temkin et al.’s observations\textsuperscript{13} that the unsteady drag of decelerating relative flows is always larger than the steady drag. The velocity distribution for this case in an inertial reference frame is shown in Fig. 7(a), and it can be seen that at t=15, the droplet almost has uniform velocities and the velocity behind the droplet is small. In comparison, Fig. 7(b) is the relative velocity distribution relative to the droplet centroid velocity at the same time. These two figures show the results for the droplet at the same instance, while the only difference is that in Fig. 7(b), the droplet centroid velocity is subtracted. It can be seen clearly from Fig. 7(b) that there is a very large recirculation region behind the deformed droplet for the Reynolds number based on the relative velocity of 24.6. This much larger recirculation region accounts for the large drag force of the droplet, which confirms the mechanism suggested by Batchelor for explaining the observations of Temkin et al.\textsuperscript{14} The proposed mechanism states that for decelerating relative flows, a larger recirculation region behind the droplet results in greater drag than that of the steady flows.

**Influence of surface tension, viscosity ratio, and density ratio**

In this section, the effects of surface tension, density ratio, and viscosity ratio on the droplet’s deformation and the drag coefficient are investigated. In order to study the effect of the surface tension, the fluids’ densities, viscosities, and the initial condition are kept constant while surface tension is varied. The value of Re_{e,j} is 40, and the viscosity and density ratios are both 50. The three initial Weber numbers are 0.4, 4.0, and 40.0. Figure 8(a) shows the effect of surface tension on the deformation of the droplets. The droplet with \(\text{We}_{e,j}\) of 0.4 shows oscillatory deformation, which was also observed

FIG. 8. Surface tension effects. (a) Deformation; (b) drag coefficient.
in previous numerical simulations for small Weber number.\textsuperscript{11,12} For the droplets with \( \text{We}_{\text{g,i}} \) of 4.0 and 40.0, due to the impulsive force from the gaseous flow initially exceeding the surface tension force, the droplets are deforming continuously. The droplet deforms more for the smaller surface tension case, which can be seen in Fig. 8\textsuperscript{a}. The effect of the surface tension on the drag coefficient is shown in Fig. 8\textsuperscript{b}. For the larger initial Weber number cases, the drag coefficients are greater. The increase in total drag for the larger \( \text{We}_{\text{g,i}} \) case indicates that momentum transfer for the larger \( \text{We}_{\text{g,i}} \) case is faster than that for the case with smaller \( \text{We}_{\text{g,i}} \). It can also be concluded that the drag coefficient depends largely on the deformation, which agrees with Hsiang et al.’s experimental observation.\textsuperscript{8} The drag coefficients of the case with \( \text{We}_{\text{g,i}} \) of 0.4 are also plotted in Fig. 6, and it can be seen clearly that for this small Weber number case, the drag coefficients agree well with the experimental results.

The effect of the viscosity ratio on the droplet dynamics is studied by increasing the droplet viscosity. The surface tension coefficients for the simulations and the gas flow free stream velocity are the same for all the simulations, and the viscosity ratios are 50 and 100, respectively. The results are shown in Figs. 9\textsuperscript{a} and 9\textsuperscript{b}. The droplet with higher viscosity deforms less than the one with lower viscosity, and this indicates that the viscous forces in the liquid droplet tend to inhibit the droplet deformation. Taylor\textsuperscript{25} and Hinze\textsuperscript{26} also observed this trend in their experimental work. The increase of the droplet viscosity results in a smaller total drag coefficient as a consequence of the smaller deformation. The liquid viscosity impacts the internal circulation in both transient and steady-state simulations. However, the mechanism by which viscosity affects the rate of droplet deformation is unique to transient flows. As time progresses, a low viscosity drop will quickly flatten out and produce very large drag forces.

Finally, the effect of density ratio on the droplet dynamics is studied by decreasing the droplet density. Figures 10\textsuperscript{a} and 10\textsuperscript{b} show the results for these cases. It can be seen that the effect of the density ratio on the total drag coefficient is much smaller than the influence of the viscosity ratio. However, the total drag force will be affected significantly, because the density ratio is considered in the definition of the total drag coefficient.

### Mesh dependence study

Multiphase flow simulations have a history of showing poor convergence with increased mesh resolution. Often, this is a consequence of the handling of discontinuities at the interface, where properties and the derivatives of velocity are discontinuous. In order to investigate the mesh dependence
of the present simulations, two meshes are used. One is a coarser mesh, which has 25,896 cells in total; the other is a finer mesh, which has 56,280 cells. The fluids’ properties, the surface tensions, and the free stream gas velocity are the same for these two simulations. Figures 11(a) and 11(b) show that the mesh effects on the deformation and the total drag coefficient are small. This further indicates that the results are reliable.

CONCLUSIONS

A number of numerical simulations have been performed using a moving mesh interface tracking method to study the physics of the impulsively accelerated droplets. The effects of the surface tension, the viscosity ratio, and the density ratio on the droplet dynamics are also investigated. The drag coefficients obtained are found to agree well with Temkin et al.’s experimental results, and the simulations show how the drag coefficients for unsteady droplets in a gaseous flow are different from the steady drag coefficients of a spherical droplet. The simulations further confirm Temkin et al.’s observations that, for decelerating relative flows, the unsteady drag is always greater than the steady drag at the same Reynolds number, and they also verify the mechanism suggested by Batchelor for explaining the larger drag force for the case with decreasing relative velocity. The initial Weber number and the viscosity ratio have significant effects on the droplet dynamics, while the density ratio does not. It is found that the decrease of the surface tension leads to larger deformation as well as greater drag force, and the increase of the droplet viscosity results in smaller deformation and less drag force.

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