Deformation of a droplet in a particulate shear flow

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A numerical simulation using a distributed-Lagrange-multiplier-based computational method is conducted in order to investigate the deformation and breakup of a droplet in a particulate shear flow. A level-set method is used to track the interface and model the surface tension. The results show that the presence of particles leads to larger droplet deformation and a perforation in the center of the droplet. It is found that the critical Stokes number above which a perforation occurs increases linearly with the inverse of the capillary number and viscosity ratio. © 2009 American Institute of Physics. [doi:10.1063/1.3205446]

I. INTRODUCTION

Droplet deformation and breakup occur in many industrial applications and natural processes such as combustion systems, ink-jet printers, emulsion, oil recovery, and biological cell systems. In the case of a dilute emulsion with negligible drop-drop interactions, the dynamics of a single drop provides useful information about the emulsion behavior. If a drop suspended in a second liquid is exposed to shear, it deforms and breaks into two or more fragments. Several theoretical, experimental, and numerical studies focus on the amount of shear rate required to break a drop and the size and number of the droplets generated from the breakup.

Drop deformation in a Newtonian fluid is governed by the Capillary number \( \text{Ca} \), the ratio of the viscous stretching force to the resistive force due to interfacial tension, and the viscosity ratio \( \lambda \). Below a critical Capillary number, drops retain an elongated but bounded shape, whereas above it they break up. In this paper, we consider the deformation and breakup of a droplet in a particulate shear flow. To our knowledge this is the first time this problem is considered. In this problem, not only the capillary number and viscosity ratio are pertinent dimensionless numbers but also the particle volume fraction, the droplet to particle diameter ratio, and the particle initial distribution are important. One important application of this work is the mechanical cell lysis method in which interaction and collision of glass beads and cells in a lysis chamber microfabricated in a compact disk are used to break cells and extract DNA for further applications. A cell has a membrane that has to be broken but this is neglected in this work and the cell is simply modeled as a droplet considering surface tension. This is still useful since the results can be used for other three component systems of solid particles/continuous liquid/dispersed liquid.

Theoretical studies have mostly focused on drop deformation at low Reynolds numbers. One of the earliest analyses of drop deformation was conducted by Taylor (1934) who studied the deformation of drops in hyperbolic and simple shear flows. The deformation of a viscous drop at low Reynolds number was summarized by Acrivos and Rallison. They presented theoretical calculations of steady deformation of nearly spherical drops and long slender drops, a description of boundary integral methods, and a summary of experimental studies. Stone and Leal studied the deformation and breakup of a droplet in time-dependent flows.

Vorticity of the external flow plays a critical role in the breakup of a droplet in shear flows. It has been found that if \( \lambda \) is larger than roughly 3.5 and the drop starts with a nearly spherical shape, drop breakup is not possible in a simple shear flow. However, breakup is always possible in a planar extensional flow for any viscosity ratio.

The investigation of droplet rupture is greatly aided by numerical techniques. Beaucourt et al. studied droplet breakup and relaxation utilizing a phase-field approach. Aggarwal and Sarkar studied deformation and breakup of a viscoelastic drop in a Newtonian matrix using the Oldroyd-B constitutive equation and a front-tracking method. Whereas several studies have been conducted on the deformation and breakup of a droplet, only few numerical studies address the effect of particles on the deformation and breakup of a droplet. Zinchenko and Davis considered a drop squeezing through a constriction formed by several solid particles rigidly held in space utilizing a boundary integral method. In
viscous flow are the Navier–Stokes equations, particles, and the droplet. The present work, we consider deformation and breakup of a liquid droplet in a shear flow of a suspension of solid particles.

II. NUMERICAL IMPLEMENTATION

In this study, we consider the motion of a liquid droplet in a particulate shear flow. The physical problem and the computational domain are shown in Fig. 1. The computational domain is \( \Omega \), including the surrounding fluid, the particles, and the droplet.

The governing equations for an unsteady, incompressible viscous flow are the Navier–Stokes equations,

\[
\rho \left( \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \nabla \cdot (2\mu \mathbf{D}) + \sigma \kappa \delta(\ell) \mathbf{n} + \mathbf{f} \quad \text{in} \quad \Omega,
\]

where \( \mathbf{u} \) is the velocity, and \( \rho \) and \( \mu \) are the density and viscosity of the fluids, respectively. Subscript \( i \) could represent either the surrounding fluid (the matrix), droplet, or the particle phase and \( \mathbf{D} \) is the strain-rate tensor. The third term on the right hand side of Eq. (1) represents the surface tension as a force concentrated on the interface. Here \( \sigma \) is the surface tension coefficient, \( \kappa \) is the curvature of interface, \( \delta \) is the Dirac delta function, \( \ell \) represents the distance from the interface, and \( \mathbf{n} \) corresponds to the unit normal vector at the interface; \( \mathbf{f} \) is rigidity force and is zero everywhere except in the particle domain and leads to the rigid-body motion inside the particles. The definition of \( \mathbf{f} \) is given in more detail in Refs. 14 and 15. The flow is characterized by the following nondimensional parameters:

\[
Re = \frac{\rho_d d_d^2 G}{4\mu_m}, \quad Ca = \frac{\mu_w d_d G}{2\sigma}, \quad \gamma_d = \frac{\rho_d}{\rho_m},
\]

\[
\gamma_p = \frac{\rho_p}{\rho_m}, \quad \lambda = \frac{\mu_d}{\mu_m},
\]

where \( d_d \) and \( d_p \) refer to the diameter of the droplet and particles, respectively. In general index \( m, d, \) and \( p \) refer to matrix, droplet, and particle, respectively. \( G \) is the shear rate.

The numerical solution of the incompressible unsteady Navier–Stokes equations is developed using the finite-volume method. The semi-implicit method for pressure-linked equations, developed by Patankar,\(^16\) is used to solve the pressure-velocity coupling. The time integration is accomplished using the second-order Crank–Nicolson scheme. A distributed-Lagrange-multiplier based method is utilized to account for the presence of particles.\(^14,15\) In order to track the motion of the interface of two incompressible immiscible fluids, the level-set method developed by Osher and co-workers\(^17,18\) is used (for details, see Ref. 17).

\[
\nabla \cdot \mathbf{u} = 0 \quad \text{in} \quad \Omega,
\]

FIG. 3. Oscillation of the drop with \( \text{Re}=40 \) and initial deformation proportional to the second spherical harmonic, \( f_2=0.5 \). (a) Aspect ratio of the drop: solid line is the present axisymmetric result and dashed line is the result of Basaran (Ref. 22). (b) Total volume of the drop normalized by its initial value.
A. Validation of the code

The numerical platform used here is the same as the one used in Refs. 14, 15, 19, and 20 and the code is validated for several benchmark problems involving the motion of solid particles in viscous liquids by Ardekani et al. 14, 15 Here, the following benchmark problem has been solved to check the accuracy of the computer code for the droplet deformation. Consider the axisymmetric oscillation of a liquid drop of radius $a_d$ in a dynamically inactive surrounding, i.e., a gas with negligible density and viscosity. The oscillation is due to surface tension energy and the deviation of the initial shape of the drop from the sphere which is at equilibrium. In order to have an inactive surrounding a density ratio and viscosity ratio of $\gamma_p = 1000$ has been used. In this problem, there is only one nondimensional variable, the Reynolds number,

$$\text{Re} = \frac{\sqrt{\rho_d \sigma a_d}}{\mu_d}. \quad (5)$$

The linear problem for small amplitude oscillations of inviscid drops has been solved previously and the effect of viscosity on the energy dissipation and damping of the oscillation has been calculated for small viscosities. 21

We conducted two axisymmetric simulations, one for $\text{Re}=40$ and large initial deformation of the drop, causing a nonlinear oscillation, and another for $\text{Re}=200$ and small initial deformation, approaching the linear-oscillation assumption. For the case with $\text{Re}=40$, the initial shape of the drop represents a departure from the sphere proportional to spherical harmonics with the formulation of

$$r(\theta, t = 0) = \gamma_n^{1/3} \left[ 1 + f_n P_n(\cos(\theta)) \right]$$

for $0 \leq \theta \leq \pi, \quad n = 2, 3, \ldots \quad (6)$

where $\theta$ is the angle in polar coordinates and $P_n$’s are Legendre’s polynomials. $f_n$ is the amplitude of the initial deformation. $\gamma_n$ is the normalization factor so the total drop volume is $\frac{2}{3} \pi a_d^3$. For the case of $n=2$ we have

\begin{align*}
(a) \quad t &= 1.68 \\
(b) \quad t &= 2.00 \\
(c) \quad t &= 2.53 \\
(d) \quad t &= 3.05
\end{align*}
Since for even harmonics, the drop represents double symmetry, axisymmetric calculation has been performed and only one-half of the axisymmetric domain has been simulated. The physical and computational domains are shown in Fig. 2. The simulation is carried out on an $82 \times 82$ uniform grid for a total time of about ten periods of oscillation. The ratio of the semimajor to the semiminor axis is plotted in Fig. 3 and is compared to the results by Basaran. Time is nondimensionalized by $\sqrt{\rho g d^3/\sigma}$. Also the total drop volume is shown in Fig. 3(b). There is less than 0.3% change in the drop volume in the entire simulation. The three-dimensional simulation of the same problem is also performed on a $62 \times 62 \times 62$ uniform grid and the results are compared to the axisymmetric simulation in Fig. 4.
The second simulation is carried out for $Re=200$. In this case, the initial shape of the drop is a prolate spheroid with the major semiaxis of 1.02. The simulation is performed on a $102^2$ uniform grid. The results are shown in Fig. 5 and are compared to the analytical solution for large Reynolds number and small amplitude.

III. RESULTS AND DISCUSSION

The deformation and breakup of a droplet in three-dimensional shear flow $u_i = G y_i$ is considered, where $x$, $y$, and $z$ are Cartesian coordinates and $i$, $j$, and $k$ are unit vectors. Figure 6 shows the deformation of an initially spherical droplet in a particulate shear flow. In this case $Ca=30$, $Re=100$, $p_d=1$, $d_p=1$, and particles are not wettable. The initial particle placement is another controlling parameter that affects droplet deformation and breakup. In order to reduce the complexity of the problem, the initial particle configuration is fixed as follows: The centers of the particles and droplets are at the middle of the domain in the $z$ direction. The two particles are placed around the droplet symmetrically in the $x$-$y$ plane. Initially $x_c/a_p=1.966$ and $y_c/a_p=0.753$. The domain size is $8.63 \times 5.89 \times 4.21$ of the droplet radius $a_d$.

As shown in Fig. 6, a hole in the droplet is generated as the particles come closer. The particles rotate around each other as they contact and the hole enlarges. Finally, the particles separate from each other. The droplet edge curls so that the droplet has a shape similar to curled tongue. In order to explain this specific shape, we plotted velocity vectors and contour plots of the $x$ component of vorticity vector in the
y-z plane at $x=1.485a_p$ and $t=3.05$ in Fig. 7. Time is nondimensionalized by $1/G$. The solid line shows the droplet interface. Two counter-rotating vortices are observed in the wake of the particles, thus the velocity is toward $+y$ near the edges of the droplet and toward $-y$ in the center. Therefore, the droplet edges are curled upward. Numerical tests were conducted to show that the motion of the particles and the droplet is independent of mesh size and time step. In Fig. 8, the $u$ and $v$ components of the particle velocity (corresponding to the top particle) as functions of time are plotted for cases with different time steps and mesh sizes. The results show that the particle velocity (nondimensionalized by $a_p G$) is independent of time step and mesh size. The deformation of a droplet with the same properties in a simple shear flow is shown in Fig. 9. The droplet is spherical at $t=0$ and it elongates and flattens as time passes. Comparing this with Fig. 6(b), we conclude that the hole observed in a droplet moving in a particulate shear flow is due to the presence of the particles and their motion only. As particles approach each other, the fluid is squeezed out of the gap region and the droplet thickness decreases in the center so that a hole is generated.

Figures 10(a)–10(c) show the deformation of a droplet in a particulate shear flow with the same characteristic described above. The only difference is that here the particles are closer in the $y$ direction and are initially located at $x_c/a_p=1.967$ and $y_c/a_p=0.33$. The perforation occurs later than in the previous case and the droplet deformation is qualitatively different. The droplet edges are curled in the opposite direction as compared to the previous case and the droplet tips are flattened.

In Figs. 11(a)–11(c), the particles and the droplet have the same characteristics as in the first two cases except that now the particles are further away in the $y$ direction and are initially located at $x_c/a_p=1.567$ and $y_c/a_p=1.33$. The droplet is flattened and elongated. In this case, the droplet has a shape similar to a surf board and no hole appears in the center of the droplet. However, the droplet deformation is larger than in the other two cases with smaller $y_c$.

Figure 12 compares the droplet deformation and hole size in all of the above cases. The dimensionless major axes are plotted as functions of time. The droplet shape does not remain ellipsoidal due to the presence of particles. We define the major axis $L$ as the diameter of the smallest sphere that contains the droplet. As it can be seen in Fig. 12, the effect of the particles on the evolution of $L$ is small. The smallest growth of the major axis occurs in the absence of the particles and the largest growth of the major axis occurs in the case when the particles are the furthest apart in the $y$ direction, corresponding to Fig. 11. However, this behavior is not
monotonic since the droplet does not feel the effect of the particles when they are far away and the droplet deformation will be similar to the case without any particles. The hole diameter $d_h$ is defined as the size of the opening in the $x$-$y$ cross section of the droplet. No perforation occurs in the case of a droplet deforming in simple shear flow. A hole develops in some cases when particles are introduced and it can grow as large as half the droplet initial diameter.

Figure 13 shows the deformation of a droplet with $\text{Ca}=0.1$, $\text{Re}=10$, $\gamma_p=1$, $\gamma_d=2$, $\lambda=100$, and $d_d/d_p=1$. Initially $x_c/a_p=1.966$ and $y_c/a_p=0.753$. Deformation of an equivalent droplet in simple shear flow is shown in Fig. 14. This droplet does not breakup in either simple shear flow or particulate shear flow. However, a larger deformation is observed in the presence of particles. No hole is generated in this case due to the small Capillary number, large surface tension, and large viscosity ratio and particles rotate around the droplet.

Figure 15 shows the deformation of a droplet with $\text{Ca}=0.025$, $\text{Re}=80$, $\gamma_p=1$, $\gamma_d=1$, $\lambda=0.2$, and $d_d/d_p=1$. Initially $x_c/a_p=3.016$ and $y_c/a_p=0.753$. The deformation of an equivalent droplet in simple shear flow is shown in Fig. 16. This droplet does not breakup in simple shear flow. However, a hole is generated in the center of such droplet in a particulate shear flow. As the particles approach each other, the fluid is squeezed out of the gap and the droplet is squashed in the center. Even though the Capillary number here is lower than in the previous case, a hole is generated in the center of the droplet. This highlights the fact that the Reynolds number and viscosity ratio also play an important role on the hole generation process.

We can now summarize the above results and understand the criterion under which the perforation occurs. One could argue that the Stokes number is more appropriate here as compared to the Reynolds number since the inertia of the particle is also important in the generation of the hole. Thus, we define the Stokes number as $\text{St}=\frac{1}{9} \times \{\rho_p d_p g y_c \cos[\sin^{-1}(y_c/a_p)]/\mu_m\}$. Consider two particles in a shear flow in the absence of a droplet. If the particles collide, the Stokes number is larger than zero, otherwise it is zero and no perforation occurs. This is compatible with the results shown in Fig. 11 in which no perforation occurs and $\text{St}=0$. The Stokes number corresponding to Fig. 6 is larger than the one corresponding to Fig. 10 which explains why a perforation occurs earlier.

As particles rotate around the droplet, all the forces along $y$ direction should balance the acceleration of the particle in the $y$ direction. A surface tension force proportional to $\sigma d_p$, a drag force proportional to $6 \pi \mu_m d_p V$, and a droplet resistance against deformation proportional to the droplet viscosity are experienced by the particles and results in their acceleration. Thus, the critical Stokes number above which a perforation occurs increases linearly with the inverse of the capillary number and viscosity ratio as $\text{St}^*=C_1+C_2(1/\text{Ca})+C_3\lambda$, where $C_1$, $C_2$, and $C_3$ are functions of $y_c/a_p$ and $d_d/d_p$. The Stokes number as a function of the inverse of the capillary number and viscosity ratio is plotted for different cases in Figs. 17(a) and 17(b). As predicted above, a straight line divides the regions so that a perforation occurs above this line.

IV. CONCLUSIONS

A numerical simulation using a finite-volume algorithm has been conducted in order to simulate the deformation and breakup of a droplet in a particulate shear flow. The results show that the presence of particles leads to a larger droplet deformation. In some cases a perforation occurs in the center of the droplet as particles approach toward each other which could lead to a faster breakup. It is shown that the Stokes number is the pertinent dimensionless parameter in this problem and the critical Stokes number above which a perforation occurs increases linearly with the inverse of the capillary number and viscosity ratio.
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