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# Dynamics of a compound droplet in shear flow

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ABSTRACT

The deformation dynamics of a compound liquid droplet in shear flow is numerically investigated in two- and three-dimensional space. The computational model is based on the immersed boundary method. This accurately and efficiently tracks the interfaces of immiscible multi-phase fluids. We extend a recently developed volume-conserving immersed boundary method for two-phase fluid flow to ternary compound droplet flows. For long time simulations, we also apply a surface remeshing algorithm. Chorin's projection method is employed, and the resulting system of discrete equations is solved by a multigrid technique. We study the effects of radius, interfacial tension ratios, and inner droplet location on the deformation of a compound droplet, and compute the inclination angles of inner and outer droplets. Simulation results indicate that the angle of the inner droplet is always greater than or equal to that of the outer one. The effect of wall confinement on compound droplet deformation is compared with that of a simple droplet. The result shows that the more confined the wall is, the more different the compound and simple droplets' behavior.

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## 1. Introduction

The dynamics of multiphase droplets is of great interest in many fields of science and technology. The hydrodynamics of simple droplets and blends under various flow conditions has been intensively investigated from theoretical (Hinch and Acrivos, 1980; Taylor, 1934), computational (Renardy and Cristini, 2001; Renardy, 2007; Janssen and Anderson, 2007; Vananroye et al., 2008; Yue et al., 2004, 2006; Pillapakkam and Singh, 2001; Sheth and Pozrikidis, 1995; Hua et al., 2013), and experimental (Rumscheidt and Mason, 1961; Torza et al., 1972; Bartok and Mason, 1959) perspectives. The growing interest in the generation and manipulation of compound droplets is mainly due to microfluidic applications (Utada et al., 2005; Chen et al., 2007; Hirofumi et al., 2007). For example, Utada et al. (2005) fabricated double emulsions that contained a single internal droplet in a core–shell geometry using a microcapillary device.

Johnson and Sadhal (1985) reviewed the fluid mechanics of compound multiphase droplets in the static state and their translation in quiescent flow. The behavior of double emulsion droplets in extensional flows was analytically studied in (Stone and Leal, 1990), and Bazhlekov et al. (1995) numerically studied the unsteady motion of a rising compound droplet in a viscous fluid under the effect of gravity using the finite element method. Smith et al. (2004) investigated the deformation and breakup of an encapsulated droplet in shear flow using the level set method. They focused on the recovery behavior of an equiviscous compound droplet, and presented a phase diagram to describe the morphologies for a range of capillary numbers and surface tensions. As a first step to develop a model for the deposition of a cell-encapsulating droplet, Tasoglu et al. (2010) studied the impact and spreading of a compound viscous droplet on a flat surface using the front-tracking method. Gao and Feng (2011) developed a diffuse-interface method to simulate the spreading and breakup of a compound drop on a partially wetting substrate. They observed three regimes for the interfacial behavior, mainly depending on the size of the inner droplet. Recently, Qu and Wang (2012) studied the hydrodynamics of concentric and eccentric compound droplets in extensional flows using the spectral boundary element method. They explored parameter effects in detail, including the relative size and surface tension of two interfaces, the capillary number, and the initial location of an inner droplet in the compound droplet, on the deformation and stability of the compound droplet in the Stokes flow regime. There are several experimental (Vananroye et al., 2007; Sibillo et al., 2006) and numerical (Renardy, 2007; Janssen and Anderson, 2007; Vananroye et al., 2008) results for the confinement effect on the

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steady-state shape of a simple droplet under shear flow. The phenomenological models make an important contribution to our comprehension of the deformation and breakup of a single droplet (Minale, 2008, 2010). However, there are no numerical results for the wall effect with respect to a compound droplet.

The novel contributions of this study are as follows: (i) we extend the three-dimensional volume-conserving immersed boundary method and apply surface remeshing for a compound droplet; (ii) the influence of fluid properties, droplet size, and inner droplet location are investigated; and (iii) the wall confinement effect is also studied and compared with a simple droplet. The rest of the paper is organized as follows. In Section 2, the mathematical governing equations are introduced. In Section 3, we describe the numerical implementation in detail. The results of numerical simulations are presented in Section 4. Finally, conclusions are drawn in Section 5.

## 2. Governing equations

We study the two- and three-dimensional dynamics of a compound liquid droplet suspended in an ambient fluid between two parallel plates under a shear flow with shear rate $\dot{\gamma}$, as schematically illustrated in Fig. 1. The domains $\Omega_1$, $\Omega_2$, and $\Omega_3$ represent the inner, outer, and ambient fluids, respectively, and $\Gamma_m$ denotes the interface between fluids $\Omega_m$ and $\Omega_{m+1}$ $(m = 1, 2)$. $\sigma_m$ is the surface tension coefficient on $\Gamma_m$, and $\rho_m$ and $\mu_m$ are density and viscosity, respectively, in $\Omega_m$. For simplicity, we consider constant density and viscosity.

In each fluid, the Navier–Stokes and continuity equations are satisfied

$$\rho_m\left(\frac{\partial \mathbf{u}_m}{\partial t} + \mathbf{u}_m \cdot \nabla \mathbf{u}_m\right) = -\nabla p_m + \mu_m \Delta \mathbf{u}_m, \quad \text{for } m = 1, 2, 3, \tag{1}$$

$$\nabla \cdot \mathbf{u}_m = 0, \tag{2}$$

where $\mathbf{u}_m = \mathbf{u}_m(\mathbf{x}, t)$ is the fluid velocity and $p_m = p_m(\mathbf{x}, t)$ is the pressure field, defined for the Cartesian coordinate $\mathbf{x} \in \Omega_m$ at time $t$. The velocity is continuous across the droplet interface $\Gamma_m$, and the normal stress jump is balanced by the interfacial force $\mathbf{f}_m$, i.e., $[-p\mathbf{I}\mathbf{n}_m + \mu\nabla\mathbf{u}\mathbf{n}_m]_{\Gamma_m} + \mathbf{f}_m = 0$, where $\mathbf{n}_m$ is the unit normal vector on $\Gamma_m$. However, it is not easy to solve Eqs. (1) and (2) directly with jump conditions at the interfaces. To overcome these difficulties, we use the immersed boundary method (IBM), which was developed by Peskin (1977). In IBM, we treat the interface as an immersed boundary that exerts a force $\mathbf{f}$ on the fluids and moves with the local fluid velocity (Lai et al., 2008).

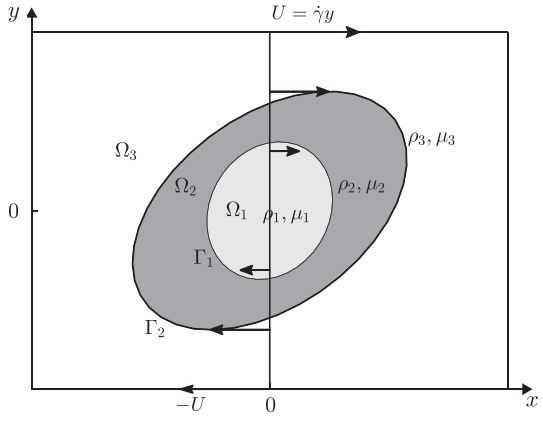


**Fig. 1.** Compound droplet in an ambient fluid under shear flow.

We denote by $\mathbf{X}_m(t)$ the Lagrangian variable for the immersed boundary $\Gamma_m, m = 1, 2$. The fluid flow is computed in the whole domain, and then $\mathbf{X}_m(t)$ is moved according to the interpolated fluid velocity. The fluid interacts with the interface through the surface tension force exerted by the boundary. This surface tension force is spread to the surrounding Eulerian variable $\mathbf{x}$ using a delta function. Then, the dimensionless equations of motion for the system of immiscible three-phase fluid flow can be written in the following form:

$$\frac{\partial \mathbf{u}(\mathbf{x}, t)}{\partial t} + \mathbf{u}(\mathbf{x}, t) \cdot \nabla \mathbf{u}(\mathbf{x}, t) = -\nabla p(\mathbf{x}, t) + \frac{1}{Re}\Delta \mathbf{u}(\mathbf{x}, t) + \mathbf{f}(\mathbf{x}, t), \tag{3}$$

$$\nabla \cdot \mathbf{u}(\mathbf{x}, t) = 0, \tag{4}$$

$$\mathbf{f}(\mathbf{x}, t) = \sum_{m=1}^{2} \frac{1}{We_m} \mathbf{f}_m(\mathbf{x}, t), \tag{5}$$

$$\mathbf{f}_m(\mathbf{x}, t) = \int_{\Gamma_m} \mathbf{F}_m(\mathbf{X}_m(t))\delta(\mathbf{x} - \mathbf{X}_m(t))ds, \tag{6}$$

$$\frac{d\mathbf{X}_m(t)}{dt} = \mathbf{U}_m(\mathbf{X}_m(t)) \quad \text{for } m = 1, 2, \tag{7}$$

$$\mathbf{U}_m(\mathbf{X}_m(t)) = \int_{\Omega} \mathbf{u}(\mathbf{x}, t)\delta(\mathbf{x} - \mathbf{X}_m(t))d\mathbf{x}. \tag{8}$$

Here, $\mathbf{u}(\mathbf{x}, t)$, $p(\mathbf{x}, t)$, $\mathbf{f}_m(\mathbf{x}, t)$ are Eulerian variables and $\mathbf{F}_m(\mathbf{X}_m(t))$, $\mathbf{U}_m(\mathbf{X}_m(t))$ are Lagrangian variables in the Cartesian domain $\Omega \subset \mathbb{R}^d$ ($d = 2$ or 3). The Lagrangian force density is defined as $\mathbf{F}_m(\mathbf{X}_m(t)) = \kappa_m(\mathbf{X}_m(t))\mathbf{n}_m(\mathbf{X}_m(t))$, where $\kappa_m$ is the mean curvature and $\mathbf{n}_m$ is the unit outward normal vector at the interface $\Gamma_m$. $\delta(\mathbf{x})$ is the Dirac delta function defined as the product of one-dimensional Dirac delta functions, i.e., $\delta(\mathbf{x}) = \delta(x)\delta(y)$ and $\delta(\mathbf{x}) = \delta(x)\delta(y)\delta(z)$ in two and three dimensions, respectively.

Let $R_1$ and $R_2$ be the undeformed radii of the inner and outer droplets, respectively. The length scale is $R_2$. $1/\dot{\gamma}$ is the time scale, where $\dot{\gamma}$ is the shear rate. Thus, $\dot{\gamma}R_2$ is the velocity scale. We now define the capillary numbers $Ca_m = \mu_3\dot{\gamma}R_m/\sigma_m$ for the inner $(m = 1)$ and outer $(m = 2)$ droplets. Other dimensionless parameters are the Reynolds number $Re = \rho_3\dot{\gamma}R_2^2/\mu_3$ and the interface-specific Weber numbers $We_m = Ca_m Re$. For the computational domains, we use $\Omega = (-L_x, L_x) \times (-L_y, L_y)$ and $\Omega = (-L_x, L_x) \times (-L_y, L_y) \times (-L_z, L_z)$ for two- and three-dimensional spaces, respectively. The initial conditions are $(u, v) = (y, 0)$ and $(u, v, w) = (z, 0, 0)$. The boundary conditions are $u(x, L_y) = -u(x, -L_y) = L_y$, $v(x, L_y) = v(x, -L_y) = 0$, and $u(x, y, L_z) = -u(x, y, -L_z) = L_z$, $v(x, y, L_z) = v(x, y, -L_z) = w(x, y, L_z) = w(x, y, -L_z) = 0$. For the pressure field, we take the homogeneous Neumann boundary condition at the top and bottom plates. In the other directions, we use periodic boundary conditions.

## 3. Numerical solution

In this section, we briefly describe the numerical solutions for IBM in three dimensions. Volume-conserving and remeshing algorithms are used to preserve the mass of the droplet and maintain a high-quality surface mesh.

### 3.1. Discretization

We discretize the domain $\Omega = (-L_x, L_x) \times (-L_y, L_y) \times (-L_z, L_z)$ in three-dimensional space. Two-dimensional discretization is analogously defined. Let the computational domain be partitioned into a uniform mesh with a space step of size $h$ in a Cartesian geometry. The center of each cell is located at $\mathbf{x}_{ijk} = (x_i, y_j, z_k)$, where

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