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Fluid Dynamics and Transport Phenomena

Asymmetric breakup of a droplet in an axisymmetric extensional flow☆

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ABSTRACT

The asymmetric breakups of a droplet in an axisymmetric cross-like microfluidic device are investigated by using a three-dimensional volume of fluid (VOF) multiphase numerical model. Two kinds of asymmetries (droplet location deviation from the symmetric geometry center and different flow rates at two symmetric outlets) generate asymmetric flow fields near the droplet, which results in the asymmetric breakup of the latter. Four typical breakup regimes (no breakup, one-side breakup, retraction breakup and direct breakup) have been observed. Two regime maps are plotted to describe the transition from one regime to another for the two types of different asymmetries, respectively. A power law model, which is based on the three critical factors (the capillary number, the asymmetry of flow fields and the initial volume ratio), is employed to predict the volume ratio of the two unequal daughter droplets generated in the direct breakup. The influences of capillary numbers and the asymmetries have been studied systematically in this paper. The larger the asymmetry is, the bigger the one-side breakup zone is. The larger the capillary number is, the more possible the breakup is in the direct breakup zone. When the radius of the initial droplet is 20 μm, the critical capillary numbers are 0.122, 0.128, 0.145, 0.165, 0.192 and 0.226 for flow asymmetry factor $A_S = 0.05$, 0.1, 0.2, 0.3, 0.4 and 0.5, respectively, in the flow system whose asymmetry is generated by location deviations. In the flow system whose asymmetry is generated by two different flow rates at two outlets, the critical capillary numbers are 0.121, 0.133, 0.145, 0.156 and 0.167 for $A_S = 1/21$, 3/23, 1/5, 7/27 and 9/29, respectively.

1. Introduction

In the dispersion process of immiscible liquids, the breakup of drops plays a critical role to determine the size distribution of drops. This issue is of major importance in heterogeneous reactions, liquid–liquid extractions, oil–water separation, emulsion polymerization and other applications that require multiphase mixing [1–3]. Thus, a better understanding of the physical mechanisms of drops breakup would be very important for these unit operations in chemical industries. It will be helpful to solve the problems involving mass transfer and heat transfer between different phases, especially, it is critical to predict the drop size distribution.

Since the pioneer work by Taylor [4] who invented the four-roll mill to generate flow fields to study the rheology of a single droplet, extensive researches have been done to investigate, theoretically, experimentally and numerically, the deformation and breakup of droplets under the shears of external flows both in infinite media and in confined geometries [5–10]. Among these works, infinite extensional flows [5–7] and hyperbolic flows in cross hydrodynamic traps [8] are employed to study the effects of viscosity ratios, interfacial tensions and capillary numbers Ca on the deformation and breakup since droplets trapped at the stagnant points are naturally deformed by the flow shears. When Ca is below a critical value Ca_c, the droplet will finally reach an equilibrium shape; when $Ca > Ca_c$, the droplet will break up into two daughter droplets.

However, most of the works concentrate on symmetric deformation and breakup [5,6,11]. Actually, asymmetric deformation and breakup always occur naturally in the macroscopic dispersion of immiscible liquids in a stirred tank. Even in an experiment which particularly studies the rheology of a single droplet in a symmetric flow field, it is very hard to locate (keep) the droplet at the exact balance point [4,12]. Recently, droplet-based microfluidics (also called digital microfluidics) technology has been developed rapidly, whose major advantage is to generate droplets with monodispersity [13]. Based on these droplets, diverse precise manipulations could be done in order to achieve various purposes, such as the fabrication of nonspherical polymer particles, microcapsules, spherical photonic crystals, and so on [14, 15]. In 2004, Link and co-workers [9] successfully broke the droplet into two daughter droplets with unequal sizes through T-junctions with two side arms of unequal lengths, which verified very well that the asymmetric geometry of microchannels could generate an asymmetric flow field and result in the asymmetric deformation and breakup of droplets. After that, various devices have been

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designed to study the asymmetric rheology behaviors of droplets in confined geometries, such as bifurcating channel [16], asymmetric T junction [17], Y junctions [16], obstacles [18,19] *etc.* In 2013, Salkin and co-workers [20] investigated the fragmentation of isolated slugs against rectangular obstacles and asymmetric loops. They found that a critical capillary number (Ca_c) was needed to break a slug. Only above Ca_c, the slug could be broken into two small daughter slugs. A mean-field approximation was introduced to predict the volume ratio of the two daughter slugs.

Along with the rapid development of computer technology, numerical simulation has become a powerful tool to study the complex fluid dynamics of droplet-based microfluidics over the last few decades [21–25]. Among various numerical methods, volume of fluid (VOF) model has been widely employed to simulate the generation and breakup of droplets in microchannels due to the simple but accurate way for dealing with topological changes of the interface in the calculation of three-dimensional flows [26,27]. Sang and co-workers [26] developed a numerical (VOF) and an analytical model to study the viscosity effect of the continuous phase on drop formation in a T junction in 2008. The prediction of drop sizes by using the analytical method shows a satisfactory agreement to the numerical result. In 2011, Bedram and Moosavi [28] successfully employed VOF model to investigate the breakup of mother drops to generate unequal daughter droplets in an asymmetric T junction with arms of different cross-sections. The numerical results were verified by comparing with an analytical theory in the limit of thin-film approximation.

Up to now, the asymmetric breakup of a droplet has not been studied systematically, especially the deep understanding of physical mechanisms. Recently, Wang and Yu [29] proposed a power law model to predict the volume ratio of the two unequal daughter droplets. Thus, based on their works, the volume of fluid (VOF) model in the commercial software FLUENT is used to investigate the asymmetric breakup of a droplet suspended in an asymmetric and axisymmetric flow field generated in a 3-dimensional (3D) cross-like micro-device in this paper. The asymmetry of the flow system is produced by putting the droplet at a position deviating from the balance point or by controlling the volume flow rate of the left and right exits.

2. Mathematical Formulations

2.1. Numerical model

The governing equations that include the equation of continuity, the equation of motion and the volume fraction equation for two-phase flows are written as follow:

$$\frac{\partial \rho}{\partial t}+\nabla\cdot(\rho \boldsymbol{v})=0 \tag{1}$$

$$\frac{\partial(\rho\boldsymbol{v})}{\partial t}+\nabla\cdot(\rho\boldsymbol{v}\boldsymbol{v})=-\nabla\boldsymbol{p}+\nabla\cdot\left[\mu(\nabla\boldsymbol{v}+\nabla\boldsymbol{v}^{\mathrm{T}})\right]+\rho\boldsymbol{g}+\boldsymbol{F} \tag{2}$$

$$\frac{\partial a_{\mathrm{d}}}{\partial t}+\boldsymbol{v}\cdot\nabla a_{\mathrm{d}}=0. \tag{3}$$

In these equations, ρ is the volume averaged density defined by Eq. (4), $\boldsymbol{v}$ is the velocity, μ is the volume averaged viscosity defined by Eq. (5), and $\boldsymbol{F}$ is the continuum surface force (CSF) [30] which is adopted to include the surface tension in the momentum equation and defined by Eq. (6).

$$\rho=a_{\mathrm{d}}\rho_{\mathrm{d}}+(1-a_{\mathrm{d}})\rho_{\mathrm{c}} \tag{4}$$

$$\mu=a_{\mathrm{d}}\mu_{\mathrm{d}}+(1-a_{\mathrm{d}})\mu_{\mathrm{c}} \tag{5}$$

$$\boldsymbol{F}=\sigma\frac{\rho k_{\mathrm{d}}\nabla a_{d}}{\frac{1}{2}(\rho_{\mathrm{d}}+\rho_{\mathrm{c}})} \tag{6}$$

$$k_{\mathrm{d}}=\nabla\cdot\hat{\boldsymbol{n}}=\nabla\cdot\frac{\boldsymbol{n}}{|\boldsymbol{n}|}=\nabla\cdot\frac{\nabla a_{\mathrm{d}}}{|\nabla a_{\mathrm{d}}|} \tag{7}$$

where ρ_d and ρ_c are densities of the dispersed and continuous phase, a_d is the volume fraction of the dispersed phase, μ_d and μ_c are viscosity of the dispersed and continuous phase, σ is the interfacial tension and k_d is curvature calculated from the divergence of the unit surface normal (Eq. (7)).

A transient, three-dimensional multiphase model in the commercial software FLUENT is employed. The PISO (Pressure-Implicit with Splitting of Operations) algorithm is used for pressure–velocity coupling. Spatial discretization terms were set as follows: the PRESTO! method for the pressure term, second order upwind for the momentum equation, and the Geo-Reconstruction scheme for the volume fraction.

2.2. Validation of the numerical method

The numerical model is first verified for Newtonian fluids by comparing the predicted results about the deformation of an initially spherical droplet in an axisymmetric extensional flow to those obtained by Stone and Leal [31].

The axisymmetric extensional flow is defined by

$$\boldsymbol{u}^{\infty}=\frac{Ca}{2}\begin{pmatrix}1&0&0\\0&1&0\\0&0&-2\end{pmatrix}\boldsymbol{x} \tag{8}$$

where the capillary number $Ca = Ga\mu_c/\sigma$. G is the shear rate, a is the radius of the initially droplet, and σ is the stress tensor. Deformation parameter $D = (L - S)\,/\,(L + S)$ is employed to describe the deformation of a droplet, where L and S are the half-length and half-width of the droplet, respectively. In addition, viscosity ratio: $\lambda = \mu_d/\mu_c$, was defined.

As shown in Fig. 1, the predicted results (circles and stars) are very consistent to those obtained by Stone and Leal [31] for both $\lambda = 1$ and $\lambda = 0.1$, which verified the validity of the numerical model.

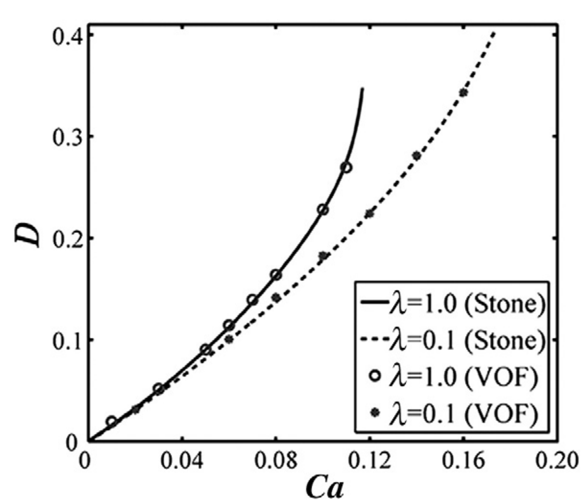

Fig. 1. Drop deformation in a steady axisymmetric extensional flow: *D versus Ca*. The open circle symbols and solid line represent our results through VOF method and those of Stone [31] for viscosity ratio $\lambda = 1$, respectively. The stars and dashed line represent our results through VOF method and those of Stone for viscosity ratio $\lambda = 0.1$, respectively.