Motion and deformation of immiscible droplet in plane Poiseuille flow at low Reynolds number[*]

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Abstract: Droplet migration in plane Poiseuille flow is numerically investigated with a dissipative particle dynamics method. The single droplet deformation in the channel flow is first studied to verify the current method and the physical model. The effect of the viscosity ratio between the droplet and the solvent and the effect of the confinement are systematically investigated. The droplet is in an off-centerline equilibrium position with a specific selection of the parameters. A large viscosity ratio makes the droplet locate in a near-wall equilibrium position, and a large capillary number makes the droplet migrate to the near-centerline region of the channel. For the droplet migration at the same Capillary number, there is a critical width of the channel, which is less than twice of the droplet diameter, and the droplet will only migrate to the channel centerline if the width is less than this critical value.

Key words: droplet, migration, particle separation, microfluidics, dissipative particle dynamics

Introduction

Microfluidics is one of the promising research areas with its potential applications in biomedicine, chemical engineering, and other fields. In the biological research, the ill and infected cells have to be isolated to detect and predict diseases at an early stage, such as cancer and blood diseases[1,2]. The properties of ill cells may change during the isolation process, including the size, the deformability or the electric properties. A properly designed microfluidics device can help to isolate different cells by utilizing hydrodynamic interactions[3]. Meanwhile, in food, pharmaceutical and material industries, it is important to have approaches to filter different size droplets and manufacture monodispersed emulsion with predictable properties[4].

From a hydrodynamic viewpoint, one of the basic mechanisms for the particle/cell separation is that the particle has an equilibrium lateral position in the channel flow due to the inertial effect. The migration of a solid particle was first studied in the 1990s and an equilibrium position between the centerline and the wall was reported. A second equilibrium position was found recently with the tube Reynolds number up to 1 000[5,6]. On the other hand, the mechanism of the cell migration is more complicated than that of the solid particle. Additional effects should be taken into account, including the deformability, the viscosity ratio, the interfacial tension as well as the viscoelasticity. The droplet suspended in another immiscible fluid can be considered as a simplified model of capsules or cells. The boundary integral method was first used to investigate the droplet motion and deformation in a parabolic flow, neglecting the inertial effect, i.e. as a Stokes flow[7,8]. The lateral migration towards the channel centerline was reported, and the size and the viscous effects were studied as well. In order to account for the inertial effect, Mortazavi and Tryggvason[9] coupled their two-dimensional Navier-Stokes solver to a front tracking algorithm to capture

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the liquid-liquid interface, and the off-centerline equilibrium position was reported in their simulation. Meanwhile, the dependences of the droplet migration on the deformation, the viscosity ratio, the periodic length, and the Reynolds number were examined. Later on, this algorithm was extended to a three-dimensional simulation[10] and the capsule migration with an elastic membrane model, i.e., as neo-Hookean material[11].

In the last decade, newly developed numerical algorithms coupled with Navier-Stokes equations were successfully applied to droplet migration studies, including the front tracking method[9], the volume of fluid method[12], and the lattice Boltzmann method[13,14]. The feasibilities of these algorithms for simulating the motion and deformation of a single droplet were demonstrated properly. However, certain phenomena in droplet hydrodynamics were seldom investigated with these algorithms, such as the droplet breakup and the coalescence of droplets. The topology of the droplet changes, which increases the complexity of these algorithms. The particle-based method might provide an alternative approach for handling these complex phenomena with their intrinsic features, without additional models being required to handle the topology variation. Recently, the dissipative particle dynamics (DPD) method was employed to study the droplet hydrodynamics, including the deformation and breakup[15] and the droplet-droplet interaction[16,17] in a linear shear flow. In this paper, we apply the DPD method to study the droplet motion and deformation in the plane Poiseuille flow, with consideration of the inertial effect, the viscosity ratio effect and the channel confinement effect. Several benchmark studies are presented, which may potentially provide insights for its applications in a wide range of droplet hydrodynamics.

1. Numerical algorithm and model

1.1 *DPD method*

The DPD method was first introduced by Hoogerbrugge and Koelman[18], and is considered as a coarse-grained approach for the molecular dynamics simulation. The motion of each DPD particle i is governed by Newton's second law of motion

$$\frac{d\boldsymbol{r}_i}{dt} = \boldsymbol{v}_i, \quad \frac{d\boldsymbol{v}_i}{dt} = \boldsymbol{f}_i \tag{1}$$

where $\boldsymbol{r}_i$ and $\boldsymbol{v}_i$ are the position and velocity vectors of particle i. Meanwhile, it is assumed that the mass of each DPD particle is unity. $\boldsymbol{f}_i$ is the summation of inter-particle forces exerted by all the other parti-

cles. Espanol and Warren[19] suggested that the inter-particle force $\boldsymbol{f}_i$ can be decomposed into three pair-wise and center-to-center forces, i.e., the conservative force, the dissipative force and the random force

$$\boldsymbol{f}_i = \sum_{j \neq i} (\boldsymbol{F}_{ij}^C + \boldsymbol{F}_{ij}^D + \boldsymbol{F}_{ij}^R) \tag{2}$$

Here, these forces will be active within a certain cutoff radius which is set to be unity as $r_C = 1$. These forces can be calculated as follows:

$$\boldsymbol{F}_{ij}^C = a_{ij}(1 - r_{ij})\hat{\boldsymbol{r}}_{ij}, \quad \boldsymbol{F}_{ij}^D = -\gamma w^D(r_{ij})(\hat{\boldsymbol{r}}_{ij} \cdot \boldsymbol{v}_{ij})\hat{\boldsymbol{r}}_{ij},$$

$$\boldsymbol{F}_{ij}^R = \sigma w^R(r_{ij})\theta_{ij}\hat{\boldsymbol{r}}_{ij} \tag{3}$$

where a_{ij}, γ and σ are the amplitudes of the conservative, dissipative and random forces, respectively. w^D and w^R are the weight functions of the dissipative and random forces, vanishing when $r_{ij} \geq r_C$. r_{ij} and $\boldsymbol{v}_{ij}$ are the relative distance and velocity between particles i and j. We also have $r_{ij} = |\boldsymbol{r}_{ij}|$ and $\hat{\boldsymbol{r}}_{ij} = \boldsymbol{r}_{ij}/r_{ij}$. θ_{ij} is the white noise, $\langle \theta_{ij} \rangle = 0$ and $\langle \theta_{ij}(t)\theta_{kl}(t') \rangle = (\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})\delta(t - t')$. According to Espanol and Warren[19], the coefficients and the weight functions in Eq.(3) should follow certain constraints to satisfy the fluctuation-dissipation theorem. In other words, if one of the coefficients and the weight functions are chosen arbitrarily and then the others should be determined by

$$w^D = [w^R]^2 \quad \text{and} \quad \sigma^2 = 2\gamma k_B T \tag{4}$$

where $k_B T$ is the Boltzmann temperature of the system. In our simulation, we adopt the weight function proposed by Fan et al.[20] to have the dynamics response of the fluid with a high Schmidt number,

$$w^D = [w^R]^2 = \left(1 - \frac{r_{ij}}{r_C}\right)^{1/2}, \quad r_{ij} < r_C \tag{5a}$$

$$w^D = [w^R]^2 = 0, \quad r_{ij} \geq r_C \tag{5b}$$

Furthermore, a large repulsive force is imposed between DPD particles from the solvent and the droplet, and hence the interfacial tension can be generated on the immiscible liquid-liquid interface. For more information of the interfacial tension, please refer to