Journal of Non-Newtonian Fluid Mechanics 212 (2014) 63–72

Contents lists available at ScienceDirect

Journal of Non-Newtonian Fluid Mechanics

journal homepage: http://www.elsevier.com/locate/jnnfm

Dissipative particle dynamics simulation of droplet suspension in shear flow at low Capillary number

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ARTICLE INFO

Article history:
Received 28 January 2014
Received in revised form 15 August 2014
Accepted 18 August 2014
Available online 27 August 2014

Keywords:
Dissipative particle dynamics (DPD)
Emulsion
Droplet deformation
Shear thinning
Viscoelastic

ABSTRACT

The dissipative particle dynamics (DPD) method is used to simulate droplet suspension. The deformation of a single droplet is first studied to validate the method and a good agreement with previous theoretical, numerical and experimental results is obtained. Droplet-droplet interaction is calibrated by simulating the process of two droplets collision. A larger repulsion force is imposed between particles from different droplet to prevent two droplets from coalescing. Dilute to semi-dilute emulsions are simulated with more than a hundred droplets suspended in another immiscible fluid. Shear thinning and non-zero normal stress differences are captured in the simulations. These phenomena are related with the mean droplet deformation parameter and mean inclination angle. The droplet deformation contributes to the increasing of suspension viscosity. Decreasing the inclination angle aligns the droplets more with the flow direction, contributing more to shear thinning. Fluid inertia increases the suspension viscosity. A good agreement is achieved between our zero shear viscosity results and previous model/experimental work.

1. Introduction

Droplets with viscosity η_d suspended in another immiscible liquid with viscosity $\eta_f = \eta_d/\lambda$, where λ is the viscosity ratio, can be considered as a simple emulsion, which has great interests and wide applications in industry, including oil-gas transportation, materials processing, food processing and pharmaceutical manufacturing [1]. Droplets can also be considered as vesicles, capsules or cells with their applications in biophysics and microfluidics [2,3]. Rheological studies on a droplet suspension can help us to understand the material properties, their non-Newtonian behaviors in relation to their microstructure.

Compared with rigid particle suspension, the rheological behavior of droplet suspensions is expected to be more complicated, due to the droplets deformation, internal flow within the droplets, droplets break up, and droplets coalescence, etc. Extensive effort has been devoted to droplet suspension or emulsion in the past few decades. Early studies with asymptotic analysis are mostly under the assumption that the droplet is spherical or nearly spherical [4–8], which is quite limited in their applications in real physical problems. With the progress in computational method and powerful computation resources, numerical simulation of complex suspensions becomes feasible, and hence the finite deformation of the droplets can be addressed properly. The boundary integral method is one of the most popular numerical methods in simulating droplet deformation in Stokes flow. It can successfully predict single droplet deformation up to its burst [9,10]. One step further, the bulk stress tensor of a very dilute emulsion or droplet suspension has been derived from the result of a single droplet deformation, see, for example, Kennedy et al. [11] As proposed by Batchelor [12], the bulk stress tensor $\mathbf{S}$ can be expressed as the contribution from the continuous-phase fluid and the dispersed-phase droplets:

$$\mathbf{S} = -P\mathbf{I} + \eta_f(\nabla\mathbf{u} + \nabla\mathbf{u}^{\mathrm{T}}) - \frac{\eta_f(1-\lambda)}{V}\int(\mathbf{un} + \mathbf{nu})dS - \frac{\Gamma}{V}\int(\mathbf{nn} - \frac{1}{3}\mathbf{I})dS, \quad (1)$$

where P is an isotropic pressure with $\mathbf{I}$ the unit tensor, $\nabla\mathbf{u}^{\mathrm{T}}$ the velocity gradient tensor of undisturbed flow, V the total volume, $\mathbf{u}$ the velocity and $\mathbf{n}$ the unit normal at the droplet surface, Γ the interfacial tension and dS the differential area of an interfacial element. (An additional term, $-\frac{1}{V}\int(\rho\mathbf{u}'\mathbf{u}')dV$, will be added once the inertial effect is considered. Here, $\mathbf{u}'$ represent the perturbation or fluctuation velocity.) In this situation, the droplet-droplet interaction is neglect. Later on, droplet-droplet interaction has been considered [13,14]. Loewenberg and Hinch [13] simulated twelve droplets with droplet volume fraction up to 30%, and the bulk stress

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http://dx.doi.org/10.1016/j.jnnfm.2014.08.011
0377-0257/

tensor was calculated with Eq. (1) as well. The shear thinning behavior and finite normal stress differences were captured. A large system with more than hundred droplets were simulated by Zinchenko and Davis [14]. However, it is difficult to take into account of non-linear effects, i.e., finite inertial, non-Newtonian rheology, with the boundary integral method. Droplets breakup and coalescence also pose a challenge for boundary integral method.

Recently, with the development of interface techniques, e.g., diffuse interface method [15], front tracking method [16] and volume of fluid method (VOF) [17], the Navier-Stokes equations were combined to simulate droplet deformation, which can fully account the viscous and inertial effects. Li and Sarkar [18] simulated a single droplet deformation in a shear flow with finite inertia. The bulk stress was also calculated using Eq. (1) and it was shown that the particle contributed stress increases when the inertia is accounted for. However, it is still a challenge for these methods to simulate the process of break up and coalescence, e.g., the algorithm would become complicated and time consuming significantly, especially in a three-dimension simulation.

In this paper, the dissipative particle dynamics method (DPD) will be used to study droplet suspension, e.g., a particle-based technique for simulating hydrodynamic behaviors. It is first introduced by Hoogerbrugge and Koelman [19], and has its basis in statistical mechanics [20–22]. Each DPD particle is regarded as a cluster of molecules modeling a behavior, undergoing a soft potential interaction with others, and hence the DPD method has a higher computational efficiency. The motions of DPD particles are governed by their Newtonian 2nd law in a continuous space. DPD system conserves both the number of particles (mass) and also the total linear momentum of the system, with both the flow kinematics and the stress tensor can be found as a part of the solution procedure. In the last two decades, DPD method has been widely applied in simulating of rigid particle suspension [19,23], polymer and long-chain molecular (DNA molecules) suspension [24], and droplet deformation [25–27] as well. In the simulation of droplet, two sets of DPD particle are used to represent two different fluid phases (suspended fluid and solvent fluid) and different particle-particle interactions are specified between particles from different phases. In this manner, it is convenient for DPD to handle the topology change of droplet, e.g., droplet break up, droplets collision and coalescence, and there is no additional function or variable is needed to describe the interface. On the other hand, as a hydrodynamic simulating technique, DPD involves both compressibility [28] and finite Reynolds number [29]. With these acknowledged and controlled, DPD is an attractive simulation method for droplet suspension. As a preliminary study, studies on single droplet deformation, two droplets collision and droplet suspension are presented in this paper. The inertial effect is considered with Reynolds number around 1. The Reynolds number does not go up further with current standard DPD method, which may cause compressible issues. Meanwhile, the properties of DPD fluid, e.g., viscosity and density, are not the input of the solver, instead, they are determined by the DPD parameters, e.g., number density and dissipative constant. As a result of this, the non-dimensional parameters, such as Reynolds number or Capillary number, can only be adjusted approximately to a exact value. Studies on single droplet deformation are well addressed in previous work and it can help us to validate our numerical method properly, while studies on droplets coalescence are still limited. Hence, in current study, phenomena of the droplet break up and coalescence are mostly avoided by keeping Capillary number less than 0.35. However, it is believed that present work may shed light on the hydrodynamic and rheological studies on droplet suspension or emulsion. In the following sections, the DPD method will be first introduced in Section 2. In Section 3, results of single deformation, two droplet collision and droplet suspension are present subsequently. Finally, the conclusion remark is given in Section 4.

2. Dissipative particle dynamics (DPD)

2.1. Overview

For the standard DPD method, the motion of a DPD particle i is governed by its Newton second law of motion,

$$\frac{d\mathbf{r}_i}{dt} = \mathbf{v}_i, \quad m\frac{d\mathbf{v}_i}{dt} = \mathbf{f}_i + \mathbf{F}^e, \tag{2}$$

where $\mathbf{r}_i$ and $\mathbf{v}_i$ are the position and velocity vectors of particle i. We assume all the DPD particles have the same value of mass m. $\mathbf{f}_i$ is the inter-particle force exerted by all the other particles and $\mathbf{F}^e$ is the external force exerting on particle i. In the framework of Español and Warren [20], the inter-particle force $\mathbf{f}_i$ contains three parts: a conservative force, a dissipative force and a random force, all are pairwise and center-to-center,

$$\mathbf{f}_i = \sum_{j\neq i}\left(\mathbf{F}_{ij}^C + \mathbf{F}_{ij}^D + \mathbf{F}_{ij}^R\right). \tag{3}$$

Here, the sum runs over all other particles within a certain cutoff radius r_C, which is usually taken as unity ($r_C = 1$). In the DPD algorithm developed by Groot and Warren [30], the conservative force $\mathbf{F}_{ij}^C$ is a soft repulsion acting along the line of centers and is given by,

$$\mathbf{F}_{ij}^C = \begin{cases} a_{ij}(1-r_{ij})\hat{\mathbf{r}}_{ij}, & r_{ij} < 1, \\ 0, & r_{ij} \geqslant 1, \end{cases} \tag{4}$$

where a_{ij} is the maximum repulsion between particle i and particle j, and $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j, r_{ij} = |\mathbf{r}_{ij}|, \hat{\mathbf{r}}_{ij} = \mathbf{r}_{ij}/|\mathbf{r}_{ij}|$. The other two forces are dissipative force $\mathbf{F}_{ij}^D$ and random force $\mathbf{F}_{ij}^R$, given by

$$\mathbf{F}_{ij}^D = -\gamma w^D(r_{ij})(\hat{\mathbf{r}}_{ij}\cdot\mathbf{v}_{ij})\hat{\mathbf{r}}_{ij}, \tag{5}$$

and

$$\mathbf{F}_{ij}^R = \sigma w^R(r_{ij})\theta_{ij}\hat{\mathbf{r}}_{ij}, \tag{6}$$

respectively. Here, γ and σ are two coefficients characterizing the strength of dissipative force and random force; $w^D(r)$ and $w^R(r)$ are the weight functions for these two forces vanishing for $r \geqslant r_C$; $\mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j$ is the relative velocity and θ_{ij} is a white noise with the properties

$$\langle\theta_{ij}(t)\rangle = 0$$

and

$$\langle\theta_{ij}(t)\theta_{kl}(t')\rangle = (\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})\delta(t-t'),$$

where $\langle\cdots\rangle$ denotes an ensemble average with respect to its own distribution function.

In order to satisfy the balance condition (fluctuation-dissipative theorem), Español and Warren [20] showed that one of the two weight functions in Eqs. (5) and (6) can be chosen arbitrarily and then the other is determined by,

$$w^D(r) = \left[w^R(r)\right]^2, \quad \text{and} \quad \sigma^2 = 2\gamma k_B T, \tag{7}$$

where $k_B T$ is the Boltzmann temperature of the system (a measure of the specific fluctuating kinetic energy of the system). In this paper, we adopt a generalized form for the dissipative weight function proposed in [24]:

$$w^D(r) = \left[w^R(r)\right]^2 = \begin{cases} (1-r/r_C)^s, & r_{ij} < r_C, \\ 0, & r_{ij} \geqslant r_C, \end{cases} \tag{8}$$

where s is exponent. In the conventional DPD system as introduced by Groot and Warren [30], it is set as $s = 2$, while in order to improve the dynamic response and increase the Schmidt number of the DPD