

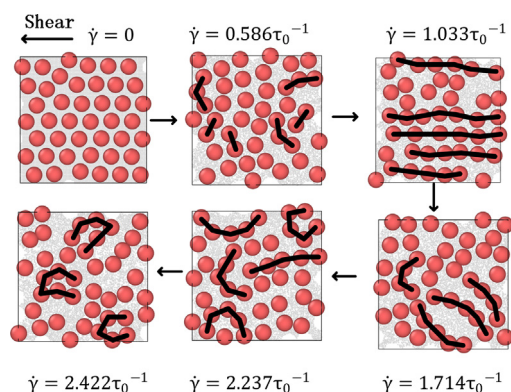
A hybrid molecular dynamics study on the non-Newtonian rheological behaviors of shear thickening fluid



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GRAPHICAL ABSTRACT



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ABSTRACT

To investigate the microstructural evolution dependency on the apparent viscosity in shear-thickening fluids (STFs), a hybrid mesoscale model combined with stochastic rotation dynamics (SRD) and molecular dynamics (MD) is used. Muller-Plathe reverse perturbation method is adopted to analyze the viscosities of STFs in a two-dimensional model. The characteristic of microstructural evolution of the colloidal suspensions under different shear rate is studied. The effect of diameter of colloidal particles and the phase volume fraction on the shear thickening behavior is investigated. Under low shear rate, the two-atom structure is formed, because of the strong particle attractions in adjacent layers. At higher shear rate, the synergetic pair structure extends to layered structure along flow direction because of the increasing hydrodynamics action. As the shear rate rises continuously, the layered structure rotates and collides with other particles, then turned to be individual particles under extension or curve string structure under compression. Finally, at the highest shear rate, the strings curve more severely and get into two-dimensional cluster. The apparent viscosity of the system changes from shear-thinning behavior to the shear-thickening behavior. This work presents valuable information for further understanding the shear thickening mechanism.

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1. Introduction

In recent year, shear thickening fluid (STF) as an added material on body armor has gained substantial attention for impact absorbers. After its impregnation into the fabric, the thickness and stiff-

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ness of the fabric show little change while the phenomenon of shear thickening (ST), which is inherent to STF, significantly enhances the ballistic resistance. ST phenomenon is one remarkable non-Newtonian rheological behavior in STF, which induces dramatic change in suspension microstructure. As a result, the viscosity will increase potentially by orders of magnitude beyond a certain shear rate. This behavior is reversible so the stress relaxes when the external shear load is removed. ST phenomenon is widely found in dense packed colloids or suspensions, which is also a concern across a range of other industrial processes involving lubricating oils, foods, powder conveying, polishing and even within the human body [1–7]. All the applications require a fundamental understanding of the complex rheological behavior of the suspension and underlying microstructure evolution during the shear flow.

The mechanism of ST behavior in colloidal suspensions has been discussed in some literatures. Hoffman [8] used light diffraction combined with shear rheology to investigate microstructural details during the ST process. He proposed an order-disorder transition, in which the flow structure changes from an ordered structure to a disordered structure, which also results in an increase in drag forces between particles. Dratler et al. [9] also thought that there was a similar transition in suspensions microstructure at the onset of ST phenomenon. However, other researchers [10–13] confirmed that under some conditions, the ST behavior could occur without order-to-disorder transition through simulation and experiments. Up to now, the most acceptable approach is the formation of “hydro-cluster” in suspensions [14–23], which is responsible for the continuous viscosity increase during the shear process and which has been observed for Brownian suspensions with moderate volume fractions. From the research results [10–23], it can be concluded that suspended particles would flow freely and get into equilibrium state at low shear-rate, then get gathered together and turn into dynamic equilibrium under higher shear rates. And yet, the link between the microstructure evolution of hydro-clusters and continuous shear thickening (CST) for non-Brownian suspensions is still a matter of debate [21]. Moreover, in contrast to a continuous viscosity increase at any applied shear rate, the discontinuous shear thickening (DST) is observed when the volume fraction of the flowing suspension is increased above a critical value. Some researchers [22–24] confirmed that the jamming of suspensions took responsible for the DST. Peter et al. [22] considered DST an independent phenomenon from shear-jammed transitions and jamming states, and they confirmed DST the conclusion of frictional contacts between particles.

Besides the discussion of the origins of ST, researchers also concerned about the influence factors on this special nonlinear behavior, such as phase volume fraction, particle size, etc. [14,25–31]. Brown et al. [30] found that increasing the packing fraction of cornstarch in water would eliminate the occurrence of ST phenomenon. Zhang et al. [31] used small fume silica (14 nm) and large particle of silica (1–5 μm) to fabricate the STF with ethylene glycol. It was found that the 14 nm silica had significant ST effect, unlike the large particle in the suspension. The DST behavior was also found dependent on the system properties, e.g., particle dispersibility or shape, as well as the flow geometry [27,28]. Even though many researchers [32–35] have demonstrated that the viscosity is firmly associated with the microstructure of colloidal particles in many solutions, there is still no direct observations of the evolution law under different influence factor of STFs and the influence mechanism of STFs is still unclear. Although many researchers have explored the STFs through Stokesian Dynamics [36], dissipative particle dynamics [37], and dynamic discrete element method [38], the evolution of microstructure of colloidal particles with ST phenomenon is still in a lack of direct observations to prove the microscopic mechanisms of STF. Therefore, a systematic investiga-

tion on this issue should be performed. Our work concerns on the relationships of transitions of microstructure and the viscosity under different shear rate in STF, so as to study the mechanism for ST phenomenon via numerical simulations.

In this work, the non-Newtonian rheological behavior of STF is studied by a hybrid model combining the molecular dynamics (MD) method and stochastic rotation dynamics (SRD) method. In the next section, we briefly review the basics of the hybrid model and the implementation of the Muller-Plathe (MP) reverse perturbation method for colloidal suspensions. The computation details are introduced at the end of this section. In Section 3, the non-Newtonian rheological behavior is studied. The relationship between the microstructural evolution and the ST behavior is analyzed. And then the influence factor on the ST behavior is discussed. Finally, the conclusion of the simulation results is drawn in the last section.

2. Simulation technique

2.1. The hybrid SRD-MD mesoscopic model

The fundamental principles of the method used here have been explained extensively elsewhere [39,40], and therefore only the most important parts will be described here. In this work, the colloidal particles are modeled with MD algorithm, while the solvent particles are simulated with SRD method. The first part of the method is the SRD method. SRD, also known as multi-particle collision dynamics (MPC), is a particle-based mesoscale simulation method for complex fluids which fully incorporates thermal fluctuations and hydrodynamic interactions. It can be seen as a “hydrodynamic heat bath”. In SRD, the solvent is modeled by a large number N of point-like particles. The multi-particle system is divided into cubic cells of regular lattices with no restriction on the number of particles in a cell. The evolution of the system consists of two steps: streaming and collision. In the streaming step, the coordinate of each particle is incremented by its displacement during the time step. Collisions are modeled by a simultaneous stochastic rotation of the relative velocities of every particle in each cell. The procedure is briefly described as followed:

Consider a set of N point particles with (continuous) coordinates $\mathbf{r}_i(t)$ and velocities $\mathbf{v}_i(t)$. During the streaming step, the i th SRD particle's position at time $n + 1$ is calculated via the simple forward Euler scheme:

$$\mathbf{r}_i^{n+1} = \mathbf{r}_i^n + \mathbf{v}_i^n \Delta t, \quad (1)$$

Δt is the value of the simulation timestep. For the collision step, particles are sorted into cells, and they interact only with the particles in their own cells. Then an independent random rotation of the relative velocities $\mathbf{v}_i - \mathbf{u}$ will be applied to the particles in each cell, where the macroscopic velocity $\mathbf{u}(\xi, t)$ is the mean velocity of the particles in the cell with coordinate ξ . The local temperature $T(\xi, t)$ is defined via the mean square deviation of the particle velocities from the mean velocity in a cell. The rotation angles of different cells are statistically independent. Throughout the process, the local momentum and kinetic energy are invariant. The velocity of i th particle at time step $(n + 1)$ during the collision step is updated from that at time step n by:

$$\mathbf{v}_i^{n+1} = \mathbf{v}_i^n + R[\xi(\mathbf{r}_i^{n+1})]\{\mathbf{v}_i^n - \mathbf{u}[\xi(\mathbf{r}_i^{n+1})]\}, \quad (2)$$

where $R[\xi(\mathbf{r}_i^{n+1})]$ denotes a stochastic rotation matrix. R is taken to be a rotation by an angle $\pm\alpha$, with probability 1/2. The value of α is set to be 90° . In every time step for each cell, one of these 6 possibilities is chosen with equal probability 1/3.

The second part of the hybrid mesoscopic method is description of dynamic behavior of the colloidal particles under the interaction

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