Migration and fractionation of deformable particles in microchannel

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The complexity of the coupling between soft particle deformation and fluid perturbation has limited studies of soft particle hydrodynamics to dilute suspensions. A hybrid Brownian dynamics-lattice Boltzmann method is presented that models nondilute soft spherical deformable particle (DP) suspensions in flow. Dependences on particle size and density are investigated for suspensions with over 100 DP. Multi-DP interactions lead to complex dependence of particle distributions on concentration and flow rate. Flow-induced DP migration toward channel center for DP in narrow channels is found. In wide channels, off-center peaks in the center of mass distribution for DP are found. The migration of DP leads to faster average speed of DP than the flow, which can be exploited for fractionating DPs of different sizes. © 2010 American Institute of Physics. [doi:10.1063/1.3457156]

I. INTRODUCTION

The dynamics of soft particle suspensions in microchannels depends on many factors and has long been a challenging problem to understand for scientists and engineers. The complex dynamics of soft particle flow is known to depend on the particle elasticity, shape, concentration, and interparticle repulsion/attraction. In applications such as microcapsule drug delivery and microfluidic droplet reactors, controlling deformable particle (DP) dynamics is critical for ensuring the transport to the intended target via microflow. In blood microcirculation, Fåhraeus in 1931 first observed that blood viscosity decreases when the flow shear rate increases in microcapillaries with certain sizes. This “shear-thinning” effect depends strongly on the diameter of the blood vessel. In addition, the dynamics of the spherical soft white blood cells are known to be coupled to the flow of the biconcave discoid elastic red blood cells (RBCs) and vice versa. To disentangle the complex interactions between different components in blood flow, models for DPs and fluid flow are needed to understand how DP-fluid, DP-vessel, and DP-DP hydrodynamic coupling affect the fluid and particle motion.

Recent studies of polymer and vesicle solutions in low Reynolds number (Re) microflow have shown that polymers also exhibit migration away from the microchannel walls. This effect has been attributed to the asymmetric hydrodynamic field produced by a contracting elastic polymer near the microchannel walls. For a deformable soft particle in solution, the competition between the particle shape-restoring elasticity, characterized by its elastic modulus $G$ and relaxation time $\tau_{\text{relax}}$, and the shear flow force, characterized by the shear rate $\dot{\gamma}$, determines the effect of particle migration. The migration force can thus be characterized by the capillary number $Ca=\dot{\gamma}n\eta/G$ or equivalently by the Weissenberg number $Wi=\dot{\gamma}\tau_{\text{relax}}$. For $Wi > 1$, the shear force overcomes the elasticity to stretch the particle. The flow field around an elastic, contracting deformable particle near the wall results in a net migration force that pushes it away from the wall. Furthermore, in studies of dense polymer solutions, the migration phenomenon is dampened by excluded volume interactions and the screening of hydrodynamic interactions. These studies suggest that manipulating the interplay between thermal fluctuations, excluded volume repulsion, and hydrodynamic interactions may allow one to exercise fine control over the flow dynamics of deformable particle suspensions.

In order to develop a model for DP suspensions in flow, one needs to account for not only how particle motion perturbs the fluid but also DP deformation due to fluid shear and hydrodynamic perturbations due to particle deformation. The pioneering boundary integral formulation of Barthès-Biesel et al. and Pozrikidis et al. extensively studied DP dynamics in capillary flow. However, accurately modeling the interplay between particle deformation and the fluid perturbations is very computationally intensive, as the DP shape and the hydrodynamic field around the DP need to be resolved simultaneously. Recent advances in the immersed boundary method, multiparticle collision method have been able to significantly improve the efficiency of complex fluid flow modeling. Extensions of these methods have allowed one to simultaneously model the dynamics of hundreds of DP, MPC and Brownian dynamics (BD)-LB have been applied to study polymers, vesicles, and RBC dynamics in flow and shown to be able to capture the behavior of red blood cell migration and vesicle tank-treading in shear flow. In this work, we investigate how the dynamics of DP suspension in flow depends on the flow rate, DP size, volume fraction, and the channel size. The deformable particle is modeled as a closed membrane and the particle dynamics is coupled to the lattice Boltzmann fluid to examine the particle distributions in dense DP suspensions and flow properties in low Reynolds number Re flow.
II. MODEL AND SIMULATION METHOD

To simulate the DP suspension, we combine the LB method and BD. LB was first used by Ahrlich and Dürenge35,36 to simulate polymer chains in solution, and a recent review explains the method in detail.30 This approach solves the fluid dynamics through the spatial propagation and temporal evolution of the discretized Boltzmann equation.31,32 The DP dynamics is modeled by using Brownian dynamics.37 The fluid and DP are coupled through exchange of the frictional momentum.

A. Fluid: Lattice Boltzmann method

The LB simulation is carried out on a three-dimensional cubic lattice with 19 discrete velocities (the D3Q9 model).34 In LB, the state of the fluid is described by the velocity distribution function \( n_i(\mathbf{r}, t) \), which is the mass density of the fluid with velocity \( \mathbf{c}_i \) at lattice site \( \mathbf{r} \) and time \( t \). The 19 velocities are given by \( \mathbf{c}_i = c/(\sqrt{3}) \left( \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0 \right) \), \( i=0 \), \( +1 \), \( -1 \), \( \pm \frac{1}{2} \), \( \pm \frac{3}{2} \), \( \pm 1 \), \( \pm 3 \). In these simulations \( e = 1 \) and \( n = 2 \).

\[
\rho = \sum n_i, \quad \rho \mathbf{u} = \sum n_i \mathbf{c}_i \mathbf{u}, \quad \Pi = \sum n_i \mathbf{c}_i \mathbf{c}_i
\]

and the equilibrium distribution can be obtained from a second-order Taylor expansion of the Maxwell–Boltzmann distribution at low-Mach number (\( \mathbf{Ma} = u/c_s \ll 1 \)).

\[
n_i^{eq} = \rho \delta^{3} \left[ 1 + \frac{\mathbf{c}_i \mathbf{u}}{c_s^2} + \frac{\mathbf{u}^2 \cdot \mathbf{c}_i^2 - c_s^4}{c_s^4} \right].
\]

For our D3Q9 system, \( a^0 = 1/3, a^1 = 1/18, \) and \( a^2 = 1/36 \). The time evolution of \( n_i \) is governed by the lattice Boltzmann equation

\[
n_i(\mathbf{r} + \mathbf{c}_i \Delta t, t + \Delta t) = n_i(\mathbf{r}, t) + \sum_j L_{ij} [n_j(\mathbf{r}, t) - n_j^{eq}(\mathbf{r}, t)] + n_i^{ext} + n_i^f,
\]

where \( L_{ij} \) is the collision operator, linearized around the local equilibrium. In the case of pressure-driven flow, a bias \( n_i^{ext} \) is added to the velocity distribution of all lattice sites.\(^{40}\) \( n_i^f \) is the fluid fluctuation added to the fluid stress.

The collision can be simplified by transforming the distributions \( n_i \) into moments \( m_k \). In the moment space, the collision operator is a diagonal matrix with diagonal elements \( \tau_k, \tau_k, \ldots, \tau_{18} \), where \( \tau_k \) is the characteristic relaxation time of moment \( m_k \). The conserved moments \( (\rho, \rho \mathbf{u}) \) and the ghost moments do not relax and \( \tau_k = 0 \). The momentum flux moments have a single relaxation time \( \tau_0 = \tau_s \). In these simulations \( \tau_s = 1 \) and the relaxation time is \( \tau_0 \Delta t \).

Through a Chapman–Enskog expansion, one can show that Eqs. (1)–(3) are equivalent to the Navier–Stokes equation in the limit of low Knudsen and Mach number.\(^{28,29}\) Low Ma requires \( u/c \ll 1/\sqrt{3} = 0.6 \). In our simulations we keep \( u/c < 0.2 \). Another condition is that the fluid relaxation time be shorter than the time fluid momentum diffuse across the system, i.e., \( \tau_0 \Delta t \ll H^2/\nu \), where \( H \) is the system size, \( \nu = \eta/\rho \) is the kinematic viscosity of the fluid, and \( \eta = \rho c_s^4 \Delta t (\tau_s - 1/2) \) is the shear viscosity of the fluid.\(^{28}\) With \( \tau_s = 1 \) this constraint leads to \( H/\Delta t \gg 1/\sqrt{6} = 0.4 \). In our simulations \( H/\Delta t = 6 \).

B. Deformable particles: Brownian dynamics

The mechanical properties of the deformable particles are modeled by accounting for the membrane elasticity. Each membrane is constructed with a collection of beads and springs. The beads interact with each other via a purely repulsive Weeks–Chandler–Andersen (WCA) potential given by

\[
U_{WCA}(r) = \begin{cases} 4\varepsilon \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^{6} + \frac{1}{4}, & r < 2^{1/6} \sigma, \\ 0, & r > 2^{1/6} \sigma. \end{cases}
\]

Neighboring beads are connected with a finite extensibility nonlinear elastic (FENE) spring, which is harmonic at small separation but restricts the separation to within \( l_0 \), given by

\[
U_{FENE}(r) = -\frac{k_0^2}{2} \ln \left[ 1 - \left( \frac{r}{l_0} \right)^2 \right], \quad r < l_0.
\]

The parameters of the potentials are chosen to be \( \sigma = \Delta x, l_0 = 3 \Delta x, \varepsilon = k_B T, \) and \( k_0 = 30k_B T \).

Bead positions on the spherical shell are acquired by triangulation, as shown in Fig. 1. The smallest sphere considered \((n=0)\) is an icosahedron, with 12 beads and 20 faces. A larger sphere \((n=1)\) can be obtained by refining each triangle of an icosahedron into four triangles, leading to 42 beads and 80 faces. The procedure can be repeated again to obtain a larger sphere \((n=2)\), with 162 beads and 320 faces. A bending force is imposed between all neighboring triangular faces

\[
U_{\text{bend}} = k_{\text{bend}} (1 - \cos \theta),
\]

where \( \theta \) is the angle between the normals of two neighboring faces, as shown in Fig. 2. \( k_{\text{bend}} = 10k_B T \) is used throughout this study to maintain the spherical shape of the shell. Together with the elastic spring force, the bending force attributes particle elasticity and relaxes particle deformations in the presence of externally applied forces.

The triangular bending force is exerted on the four beads that make up the two adjacent triangles, as shown in Fig. 2, given by

![](image)
the simulation unit of mass. The velocity Verlet method is

distributed on the particle surface

where

\( m \) and \( k \) are the mass and the stiffness, respectively. The sign of \( \theta \) is given by \( \sin \theta = (\hat{n}_x \times \hat{n}_y) \cdot \hat{e} \), where \( \hat{e} = \hat{n}_1 - \hat{n}_2 \). Equation (6) has the expected directionality for a force that only affects the angle but does not affect the translation, rotation, and shape of the two triangles.

In addition, particle volume is conserved by applying an isotropic pressure \( P_V(t) \) on the particle, given by

\[
P_V(t) = F_V(t)/A = [k_V(V(t) - V_0)/V_0]/A,
\]

where \( V(t) \) and \( V_0 \) are the dynamic and initial particle volumes, respectively. The volume constraint force \( F_V \) is equally distributed on the particle surface \( A \) on the monomers. We found that with \( k_V = 2k_BT/\sigma \), the particle volume is conserved within \( 2\% V_0 \) at the highest shear rate examined here. The total conservative force acting on each bead is given by \( F^C = -\nabla U + F_{\text{WCA}} + F_{\text{FENE}} + F_{\text{bend}} + F_V \). All beads have mass \( m_b = 36m_0 \), to be compared with \( m_p = 0.01696m_0 \), where \( m_0 \) is the simulation unit of mass. The velocity Verlet method is employed to project the bead trajectories. The Brownian dynamics time step is \( \delta t = 0.1\Delta t \).

C. Fluid-DP coupling and thermal fluctuations

The particle hydrodynamic interactions can be captured by the exchange and propagation of frictional momentum between the fluid and the DP.\(^{36,39}\) Each bead on the DP experiences a friction force

\[
F_f = -\zeta (\mathbf{u}_f(r_b) - \mathbf{u}_l(r_b)),
\]

where \( \mathbf{u}_f(r_b) \) and \( \mathbf{u}_l(r_b) \) are the bead and fluid velocity at position \( r_b \), respectively, and \( \zeta = 3\pi n\eta r \) is the bead friction coefficient. The fluid velocity at position \( r_b \) is determined by a trilinear interpolation of the fluid velocity on the neighboring lattice points \( nn \) that enclose \( r_b \), \( \mathbf{u}_f(r_b) = \sum_{x=mn} \omega_{x} \mathbf{u}(r) \), where the weights \( \omega_{x} \) are the coefficients of the normalized linear Lagrange interpolation polynomial.

In time \( \delta t \), the frictional momentum density \( \Delta j = -F_f \delta t/\Delta z^3 = \sum_{x=mn} \Delta n_x(r) \mathbf{c}_x \) is transferred to the fluid. This momentum density is distributed to the neighboring lattice sites \( nn \) with the same weight \( \omega_x \).

\[
\Delta n_x/r = w \delta_x(r) - \mathbf{c}_x, \quad r \in nn.
\]

Due to the dissipative nature of this coupling, thermal fluctuations for both the fluid and the DP are included. Fluctuation in the fluid is added to the stress tensor through a stochastic term

\[
n_x' = -\frac{\sigma_i^2}{2c_x} \sum_\alpha \sigma_{\alpha\beta}^x \delta_{\alpha\beta} \mathbf{c}_\beta, \quad \alpha = \beta = 1, 2, 3
\]

where the stress fluctuations \( \sigma_{\alpha\beta}^x \) have Gaussian distribution with zero mean and variance,

\[
\langle \sigma_{\alpha\beta}^x(r,t) \sigma_{\gamma\delta}^x(r',t') \rangle = \frac{2\eta k_BT}{\tau_3 \Delta x^3 \Delta t} \delta_{rr} \delta_{tt} \left( \delta_{\alpha\gamma} \delta_{\beta\delta} + \delta_{\alpha\delta} \delta_{\beta\gamma} - \frac{2}{3} \delta_{\alpha\beta} \delta_{\gamma\delta} \right).
\]

For the DP Brownian dynamics, the bead thermal fluctuation is given by a stochastic force \( \mathbf{f} \) with zero mean and variance,

\[
\langle f_{\alpha}(t)f_{\beta}(t') \rangle = \delta(t - t') \delta_{\alpha\beta} 2k_BT \zeta.
\]

In these simulations, \( \zeta = 56.4m_0/\Delta t \) and \( k_BT = 0.005 652m_0\Delta x^2/\Delta t^2 \), and the bead diffusivity \( D_0 = k_BT/\zeta = 10^{-4} \Delta x^2/\Delta t \).

D. Single DP properties

DP dynamics in flow depend on the particle size, elasticity, particle diffusion, and coupling with the flow field and the walls. The particle size is defined by its radius of gyration \( R_g \) given by \( R_g^2 = R_x^2 + R_y^2 + R_z^2 \), where \( R_x \leq R_y \leq R_z \) are the eigenvalues of the radius of gyration tensor. For a perfect sphere \( R_x = R_y = R_z \). The particle diffusion coefficient \( D \) is evaluated from the mean square displacement \( \langle \Delta x^2 \rangle = 6Dt \).

The particle elasticity is characterized by the elastic modulus \( G = \text{stress/strain} = f_s/\delta R_s/\delta R_0 \), where \( f_s \) is the external force per unit area of the deformed membrane. \( G \) is measured from particle deformation caused by an externally applied force. In an analogy to polymer elasticity, the particle elasticity may also be characterized by its deformation relaxation time \( \tau_{\text{relax}} \), measured from the relaxation of the particle stretch after shear deformation by fitting to \( [L(t) - L_0]^2/\tau_{\text{relax}} \sim \exp(-t/\tau_{\text{relax}}) \), where \( L \) is the deformed particle extension. Table I reports the measured values for \( G \), \( \tau_{\text{relax}} \), \( R_g \), and the DP diffusion constant \( D \). Simulations are performed using \( k_{\text{bend}}/k_BT = 10 \). As expected, the elastic relaxation time \( \tau_{\text{relax}} \) increases as the particle size increases.

The flow field of a moving DP is compared to that of a hard sphere (HS) whose boundary is defined by the bounce-
back condition. For the DP, an external force $F = f \hat{x}$ is added to each bead on the spherical shell. For HS, the external force is added to the center of the sphere. The flow field is calculated at a fixed particle position. Figure 3 compares the fluid velocity field for DP and HS in the $xy$-plane that sections the center of the sphere. The velocity fields in the fluid outside the particle agree quantitatively. Figure 4 compares the fluid velocity $u(x,y)$ along the center axis in the $xy$-plane. It is found that the flow fields produced by DP and hard sphere are equivalent in the far field region and the differences are less than 10% near the particle surface. The small quantitative differences are due to the different boundary approximations employed for DP and HS. The calculated fluid velocity profile is also in agreement with the predicted velocity field generated by a point force moving in a periodic array, given by

$$u(r) = \frac{1 + rr^2}{8 \pi \eta r} F,$$

where $r = |r|$ is the distance from the particle center. The key difference between DP and HS is that there is no fluid flow inside the hard particles, while there is fluid flow inside DP. The fluid motion inside the DP has been found to affect

<table>
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<th>Type</th>
<th>$G$</th>
<th>$\tau_{\text{rel}}$</th>
<th>$R_0$</th>
<th>$D/D_0$</th>
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<tr>
<td>$n1$</td>
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<td>1.70</td>
<td>0.18</td>
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<td>$n2$</td>
<td>3.21</td>
<td>100.0</td>
<td>3.28</td>
<td>0.08</td>
</tr>
</tbody>
</table>

FIG. 3. Fluid velocity field $u(r)$ for a single moving particle. Top: $u_x$ for DP (left) and HS (right). Bottom: $u_y$ for DP (left) and HS (right).

FIG. 4. Scaled hydrodynamic flow field of a single moving DP with radii of 3.28 ($n2$) and 1.7 ($n1$), hard particles with radius $R=3.28$ and 1.7, and a point force.
whether a DP undergoes tank-treading motion or tumbling motion under shear, depending on the shear rate and the inner fluid viscosity.\textsuperscript{1,26}

DP dynamics near a wall is further investigated by examining the hydrodynamically induced migration force away from the wall in shear flow. As seen in Fig. 5, a shear-deformed DP near the wall induces a hydrodynamic field with a net flow in the wall-normal direction away from the wall. This asymmetric DP-induced flow field near the wall leads to net DP migration toward the channel center. The effect of this wall-induced migration is further investigated in the next section.

III. RESULTS AND DISCUSSION

A. DP deformation and DP-DP interaction in shear flow

The present elastic sphere model can be validated with comparisons to theoretical predictions and experimental measurements of soft particles. The particle deformation in flow is determined by the balance between the shear force experienced by the particle and the particle elasticity, characterized by the Capillary number Ca. Particle deformation may be described with the Taylor deformation parameter as $\Delta = (L-B)/(L+B)$, where $L$ and $B$ are the longest and shortest particle principal axes, respectively. Figure 6 shows that $\Delta$ depends linearly on Ca for Ca $\ll$ 1, which agrees with the theoretical predictions\textsuperscript{17} of $\Delta = 25/4$ Ca and confirmed by experiments on polystyrene particles.\textsuperscript{43} The deformation parameter $\Delta$ oscillates sinusoidally around the theoretical prediction, confirming previous observations in experiments\textsuperscript{3,43} and numerical simulations.\textsuperscript{44}

In nondilute suspensions, interparticle hydrodynamic interactions and collisions introduce additional complexity to the flow dynamics. We examine two n2 particles in simple shear flow with $u_i = \dot{y} y$ and $u_s = u_\tau = 0$. The two particles are initially located at $(\pm x_0, \pm \delta y_0, 0)$. As the flow drives the particles toward each other, the particles are displaced by interparticle hydrodynamic interactions. Figures 7(a) and 7(b) show the trajectories of the two particle centers in simple shear flow. As the flow drives the particles toward each other, the particles are displaced by interparticle hydrodynamic interactions during the collision. It is found that at higher Ca, the particle displacement decreases, as shown in Figs. 7(c) and 7(d). As the particles collide, they push each other away through hydrodynamic interactions, and the particle centers of mass move toward the center after the collision due to the particle elastic restoration. For Ca = 0.015 with $\Delta y_0 = 0.5R_g$, the final displacement is found to be $+1.4R_g$. This is in near quantitative agreement with previous experimental studies on polymer droplets and boundary integral calculations.\textsuperscript{18,45} Furthermore, Fig. 7 shows that there is a significant difference between the particle trajectories for particles that are initially close to and far away from each other. For $\Delta x_0 = 5R_g$, the two particles appear to move closer to each other in the vorticity direction as they approach each other before the collision, which captures what was observed in prior experiments and simulations.\textsuperscript{18,45} In contrast, this "attraction" to the center is not found for $\Delta x_0 = 2R_g$ nor when the particles are initially close in the experiments. It suggests that when two particles approach each other from far away, a low-pressure region at the center of mass of the two particles pulls the particles toward each other.
B. Single component in pressure-driven flow

To study DP migration under pressure-driven flow as in microcirculation, we investigate the DP dynamics in pressure-driven flow inside a slit channel of height $H$ in the $\hat{y}$ direction and periodic boundaries in the $\hat{x}$ and $\hat{z}$ directions. The box size $W$ along the $\hat{x}$ and $\hat{z}$ directions is sufficiently large ($W > 2H$) so that hydrodynamic interaction between distant periodic images is negligible. A constant pressure is applied to the fluid along $\hat{x}$ direction, resulting in the Poiseuille flow in the slit channel.

Prior studies of polymer solutions have characterized the polymer migration phenomena in terms of the competition between the shear rate and the polymer elastic relaxation time using the dimensionless group $Wi$. For polymer solutions, the depletion layer thickness has been found to increase for $Wi > 1$, while the transient time to steady state increases with $Wi$. As the hydrodynamic mechanism for DP migration is similar to polymer migration, $Wi$ is employed to characterize the competition between particle deformation due to shear and the particle relaxation.

Several factors that affect the particle distribution function in the channel and fluid dynamics are considered: (i) the channel width, characterized by $H/R_g$. A narrow channel ($H/R_g=5$) and a wide channel ($H/R_g=10$) are considered to examine how channel confinement affects suspension dynamics. (ii) The effects of DP volume fraction $\phi=(4\pi/3) \times (N_{DP} R_g^3 / H L^2)$. It is investigated by considering a dilute ($\phi=0.03$) and a semidilute suspension ($\phi=0.15$). (iii) The flow rate, characterized by $Wi=\gamma \tau_{relax}$. Simulations with $Wi=0$, 0.25, and 1.0 are performed. The fastest flow rate corresponds to channel Reynolds number of $Re=26.7$, indicating that the fluid flow is well within the laminar flow regime. The normalized steady state particle center of mass distribution function in the channel wall cross-section, $g_c(y)$, is collected from distribution of over a hundred particles averaged over more than 2000 $\tau_{relax}$. Errors in $g_c(y)$ are estimated from the difference of $g_c(y<H/2)$ and $g_c(y>H/2)$, which are equivalent given sufficiently large statistical samples.

1. $H/R_g=5$ slits

In narrow slit channels, a single particle occupies a large portion of the parabolic flow profile and experiences hydrodynamic migration force from both wall channels. As $Wi$ increases, Fig. 8 shows that the distribution of $n_2$ particles tends to form a single sharp peak. The migration phenomenon is similar to that observed in polymer flow in confined channels and is attributed to the intrapolymer hydrodynamic interactions of a stretched polymer near a wall. At higher $\phi$, wall-particle excluded volume interaction deforms the spheres and causes the spheres to align along the wall, thus allowing closer packing away from the channel center, observed with the presence of two off-centered peaks even without flow shown in Fig. 8(b). In flow, DP migration becomes clear only for $Wi=1.0$, indicating that particles tend to spread out due to interparticle repulsion. The DP distributions in flow are broadened due to interparticle excluded volume repulsion at the channel center.

2. $H/R_g=10$ slits

In wider channels, the confinement effects are weak. The wall-induced and deformation-induced migration forces tend to push the particles toward the channel center, while the mobility gradient tends to keep the particles from the channel center. At low volume fraction, the distributions of $n_2$ exhibit double maxima at high $Wi$. When the volume fraction is higher and interparticle repulsions become stronger, the location of the two peaks is pushed toward the walls and a third peak forms at the channel center, as shown in Fig. 9(b). The distance between the central peak and the side peak is roughly equal to $2(R_g+\Delta x)$, which is the exclude volume diameter of the DP. This suggests that the center peak may be due to the interparticle packing, where the space between the two near-wall peaks allows one additional layer of particles to stay in the middle.

The competition between the mobility gradient and the migration force results in the off-center density maxima. Figure 10 shows the center of mass distribution of $n_2$ as the particles flow and migrate toward the channel center. Particle migration toward the channel center may be characterized by the thickness of the near-wall depletion layer $L_d$, where particles are depleted. In quiescent fluid, the depletion layer for the particle center of mass has the thickness of $R_g$ due to excluded volume interaction. As the particles migrate away from the wall during flow, $L_d$ increases. In addition, it is observed that the particle density is highest near the boundary of the depletion layer with maxima away from the channel center. This was also observed for polymer distribution in flow. It may be attributed to (a) the decay of the wall mi-
migration force near the center and (b) the higher mobility of particles near the channel center, where the shear rate is smaller and the particles are less deformed. The more spherical particles are able to diffuse away from the center at higher rates than the diffusion flux of deformed ellipsoids to the center.

Under the Poiseuille flow and a parabolic flow profile, the particle distribution function in channel are further investigated. As seen here, the interplay between hydrodynamic migration, the particle mobility gradient, and the entropic excluded volume repulsion leads to very rich and interesting flow dynamics.

C. Fractionation: Multiple components in pressure-driven flow

A consequence of DP migration in the Poiseuille flow is that the average DP velocity will be faster than the average fluid velocity, leading to increased DP concentration in the outflow. This is qualitatively consistent with the Fåhraeus–Lindqvist effect. In addition, when a suspension contains two different types of particles, the density distribution of the particles can change drastically and allow for particle flow fractionation. To investigate the possibility of flow fractionation and the effects of excluded volume repulsion, a suspension mixture of n0 and n2 is studied. The suspension is driven at a flow rate that corresponds to Wi=1.0 for n2. Since n0 has a smaller τrelax, Wi for n0 is =0.3.

The center of mass distribution functions are determined from five independent simulations of a mixture of φ0 =0.0059(Nn0=80) n0 particles and increasing φ2 n2 particles. Figure 11 shows that gc of n2 retains its double maxima structure for φ2 ≤0.065. As φ2 increases, the density distribution broadens and flattens out, and a small maximum is found near the center. On the other hand, the distribution of n0 remains depleted at the center with two distinct maxima inside the n2 depletion layer. As φ2 increases, the off-center maxima increase and move toward the wall, cor-

FIG. 10. Center of mass distribution for the n2 particles in a wide channel H/Rg=10, Wi=0.0 (solid line), 0.25 (square), and 1.0 (triangle) for (a) φ =0.03 and (b) 0.15. The system sizes are 68×32×64Δx3 and 64×32×64Δx3, respectively. The φ=0.03 data are collected from the average of 15 simulations of 20 particles each. The φ=0.15 data are collected from the average of five simulations of 89 particles each.

FIG. 11. Center of mass distribution in the n0+n2 mixture in flow for (a) the n0 particles and (b) the n2 particles. The simulation is performed in a 64×32×64Δx3 slit channel with a shear rate of γ=0.0043 and kBT/ξ =10−4.
responding to the broadening $n_2$ distribution. This shows that the excluded volume repulsion between $n_2$ and $n_0$ pushes $n_0$ toward the wall, which leads to slower average velocity for $n_0$.

Due to the difference in the particle density distribution in the Poiseuille flow, $n_0$ and $n_2$ flow at different average speeds. $n_2$ are present mostly at the center of the slit, where the flow speed is faster. $n_0$ particles are closer to the wall, where the flow speed is smaller. This creates a "flow fractionation" effect: The pressure-driven flow may be used to pick out the $n_2$ from the $n_0$ due to the difference in their average speed. As shown in Fig. 12(a), the average speed for $n_2$, $\langle v_r(n_2) \rangle$ is faster than $\langle v_r(n_0) \rangle$. As $N_{n_2}$ increases, the difference in speed between $n_2$ and $n_0$ increases. Figure 12(b) shows that the ratio of the speeds $\langle v_r(n_2) \rangle/\langle v_r(n_0) \rangle$ can increase from 1.3 to 2, and the velocity difference increases by threefold as $\phi_2$ increases. In addition, a mixture of $n_1$ and $n_2$ was examined and similar effects has been found. The ratio of $\langle v_r(n_2) \rangle/\langle v_r(n_1) \rangle$ also increases with $\phi_2$, although it is smaller than $\langle v_r(n_2) \rangle/\langle v_r(n_0) \rangle$ due to the fact that the elasticity of $n_1$ is closer to $n_2$, and the effective $Wi_{\phi_2}=0.6$ for $n_1$ is larger. In addition, it is found that $\langle v_r(n_2) \rangle$ in the $n_1+n_2$ mixture and $n_0+n_2$ mixture are equal when $\phi_0$ and $\phi_1$ are small.

IV. CONCLUSION

In this study, we developed a hybrid lattice Boltzmann–Brownian dynamics method for studying dense suspensions of soft, deformable particles. The DP-flow hydrodynamic interaction is verified by comparison with that of a hard sphere. The DP-DP hydrodynamic interaction is found to agree nearly quantitatively with prior experiments and simulations. LB reduces the computational cost to resolve the interparticle hydrodynamic interactions and allows for simulation of more than 100 deformable particles in a reasonable amount of time on a single workstation. For example, the BD-LB time to simulate the dynamics of 89 $n_2$ particles in a $H/R_g=10$ slit for 2000 $\tau_{relax}$ took around 4 days on an Intel Xeon Woodcrest 2.66 GHz workstation at the Institute of Physics, Academia Sinica, and the cost of the simulation increases linearly with the number of particles for a given channel size. An additional advantage is that the method is highly parallelizable for larger systems. However, the current method has limits for interbead separation, which must be larger than $\Delta x$. This may be overcome with adaptive grid methods. In addition, our current implementation does not allow for different fluid viscosities inside the particles, which will be included in the future.

Our study investigated how DP size, volume fraction, and channel size affect the dynamics of flowing DP suspensions at different flow rates and channel-to-particle ratios. It is found that (a) DP migrates toward the center of the channel due to the asymmetric hydrodynamic interactions caused by the deformation of particles near the wall. This is in agreement with previous observations of blood flow and soft particle suspensions. The competition between hydrodynamic migration and the mobility gradient leads to an off-center peak in the particle density distribution in wide channels. (b) As $\phi$ increases, the particle distributions broaden. In the case of wide channels, the particle distribution maxima move toward the wall. At sufficiently high $\phi_1$, strong interparticle repulsion can result in particle packing in the channel center. (c) DP migration leads to faster average speed of the particles that effectively reduces the viscosity of the suspension, which is in qualitative agreement with the Fåhraeus–Lindqvist effect. It is discovered that for binary mixtures, increasing the concentration of one particle species can increase the average velocity ratio between the two particle species, which leads to an improvement in separation efficiency. These results show a new mechanism for increasing the velocity ratio by more than fivefold for particles with large differences in size and deformability. Future work will further investigate the effects of particle shape and particle deformability on the particle velocity in flow, in addition to applications to blood flow and microcapsule delivery.

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Microflow migration and fractionation of DP
