Hydrodynamic interactions in dissipative particle dynamics

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Dissipative particle dynamics (DPD) has recently attracted great interest due to its potential to simulate the dynamics of colloidal particles in fluidic devices. In this work, we explore the validity of DPD to reproduce the hydrodynamic interaction between a suspended particle and confining solid walls. We first show that a relatively large Schmidt number of the DPD fluid can be obtained by increasing the ratio between the strength of the dissipative force and the kinetic energy of the particles. We then measure the mobility and diffusion coefficient of the colloidal particles and show good agreement with the predicted results. We then focus on the particle-solid interactions and measure the force on a colloidal particle moving both parallel and perpendicular to two parallel walls. In both cases we found good agreement with the theoretical predictions based on Stokes flows for separations as small as one-tenth of the particle radius. © 2008 American Institute of Physics. [DOI: 10.1063/1.2980039]

I. INTRODUCTION

Fluidics (both micro- and nanofluidics) has grown into a field that cuts across many science and engineering disciplines. A particularly important area driving the development of fluidic devices is separation sciences, leading to a renewed interest in fundamental and long-standing problems in fluid mechanics, such as the transport of suspensions in confined geometries. Novel strategies have been proposed for the separation of suspended macromolecules moving through periodic arrays of obstacles in microfluidic devices, and hydrodynamic interactions might play a crucial role in the experimentally observed size separation. It is therefore crucial to understand the dynamics of suspended particles when their size is similar to the characteristic size of the microfluidic features.

Several numerical methods are available to study the transport of suspended particles in the presence of particle-solid hydrodynamic interactions. Many of these methods, however, are not suited to describe mesoscale systems with characteristic length scales between 0.1 μm and tens of microns. For example, a fully atomistic description of the system using molecular dynamics simulations is clearly beyond computational reach. On the other hand, standard methods to solve continuum descriptions at the macroscopic level do not incorporate thermal fluctuations and might fail to describe the behavior at submicron length scales. Numerical methods that have successfully described mesoscale systems include: Brownian dynamics (BD), lattice-gas automata, and lattice Boltzmann (LB) simulations. However, they are not particularly suited for the simulation of suspended particles interacting with solid obstacles. In BD, for example, hydrodynamic interactions need to be explicitly incorporated into the forces, which is only possible in very simple geometries or for bulk suspensions as in Stokesian dynamics simulations. The uniform grids used in LB simulations pose a clear problem to simulating suspended particles in confined geometries. In fact, to accurately describe particle-solid hydrodynamic interactions at small separations, a lubrication term is typically incorporated into the LB method. In addition, thermal fluctuations would also need to be incorporated into the LB method. Here, we explore the use of dissipative particle dynamics (DPD), an increasingly popular computational method used to model complex fluid systems at the mesoscopic level. It has been shown that DPD reproduces hydrodynamic behavior consistent with the Navier-Stokes equations, much in the same way as lattice-gas and LB methods. The challenge then is to connect the results from DPD simulations to the corresponding physical regimes of interest (see a clear discussion on this issue in Ref. 23). This is especially relevant in DPD given that there is no systematic connection between the various parameters controlling the interparticle and random forces in the DPD method and the interactions present at the underlying atomistic level. Therefore, it is important to validate the DPD method as a reliable computational tool to describe the behavior of colloidal particles in fluidic devices. Previous studies have investigated the rheology of colloidal suspensions using DPD simulations. In particular, Marty's carefully compared the DPD results with theoretical predictions and found good agreement. The flow around a single sphere and through a periodic array of spheres has also been investigated using DPD simulations, and good agreement with theoretical predictions was observed. Here we focus on the hydrodynamic interactions between a colloidal particle and confining walls for the application of DPD methods in low Reynolds number flows in microfluidic systems with more complex structures, such as separation systems based on obstacle arrays.

First, in Sec. II, we briefly describe the simulation method. In Sec. III we simulate the flow of a DPD fluid in...
simple geometries and obtain the viscosity and diffusivity of the DPD fluid. Finally, in Sec. IV we measure the drag and diffusivity of single particles in bulk as well as the hydrodynamic interaction between suspended particles and solid walls, and compare these results with theoretical predictions.

II. DPD SIMULATION METHOD

The method of DPD was originally proposed as a coarse-grained method for simulating hydrodynamic phenomena, and combines ideas from molecular dynamics, BD, and lattice-gas automata. A DPD particle represents a group of atoms or molecules and is the constitutive element of both fluids and solids in the system. The effective inter-particle force between two DPD particles is typically divided into a conservative force $F^C$, a dissipative force $F^D$, and a random force $F^R$, all of which conserve the total momentum of the system (both linear and angular momenta). The conservative force is a repulsive central force, with a cutoff distance $r_c=1$,

$$F^C_{ij} = \begin{cases} a_j(1 - r_{ij}/r_c) \vec{r}_{ij}, & (r_{ij} < r_c), \\ 0, & (r_{ij} > r_c), \end{cases}$$

where $a$ is a constant that weights the repulsion between DPD particles, $r_{ij}=r_i-r_j$, $r_{ij}=|r_{ij}|$, and $\vec{r}_{ij}=r_{ij}/r_{ij}$. The dissipative force is proportional to the relative velocity between the particles, and together with the random force determines the temperature of the system,

$$F^D_{ij} = -\gamma w^D(r_{ij}) (\vec{r}_{ij} \cdot \vec{v}_{ij}) \vec{r}_{ij},$$

$$F^R_{ij} = \sigma w^R(r_{ij}) \theta \vec{r}_{ij},$$

where $\vec{v}_{ij}=\vec{v}_i-\vec{v}_j$, and the stochastic variable $\theta$ is a Gaussian white noise with zero mean and unit variance. In addition, in order to maintain a well-defined temperature that is consistent with the fluctuation-dissipation theorem and to reach an equilibrium distribution that corresponds to the canonical ensemble in statistical mechanics, the random and the dissipative forces have to satisfy the following relations:

$$\sigma^2 = 2\gamma kT \quad \text{and} \quad w^D(r_{ij}) = [w^R(r_{ij})]^2,$$

where $k$ is the Boltzmann constant and $T$ is the temperature of the system. Different formulations of $w^D(r)$ have been discussed in literature. Here, we use the standard quadratic function,

$$w^D(r_{ij}) = \begin{cases} (1 - r_{ij})^2, & (r_{ij} < r_c), \\ 0, & (r_{ij} > r_c). \end{cases}$$

The dynamics of the system is obtained by integrating Newton’s equations of motion. Here, we use the velocity-Verlet algorithm, as described in Ref. 27, with $\lambda=1/2$ and time step of $\Delta t=0.01$. Periodic boundary conditions are used whenever necessary.

A. Spherical particles and solid surfaces

The DPD method can be used to simulate not only simple fluids but also complex systems, including colloidal particles and solid surfaces. A straightforward approach to simulating solids is to use rigid assemblies of DPD particles (frozen DPD particles). Following this approach, we initially position the DPD particles on the lattice sites of a fcc solid with the desired density. Then, spherical particles and wall surfaces are constructed by freezing the DPD particles within the boundaries of the solid. Specifically, a solid sphere is made of all the DPD particles within a spherical volume of radius $R$. In the case of solid walls we use the same density of DPD particles as in the fluid, $\rho_w=\rho_f$. On the other hand, to be able to simulate smooth colloidal particles with relatively small sizes, $R \sim 1$, we use a density of solid DPD particles that is substantially larger than the fluid density, $\rho_p=27\rho_f$. In this case, a sphere of radius $R=1$ contains 453 solid DPD particles.

The solid DPD particles either remain still, inside the solid walls, or move like a rigid body, as part of the solid sphere. The force on the solid particle is computed as the sum of the forces on each constituent DPD particle, and the rigid body dynamics of the particle is integrated following standard methods. Note that the higher density of the DPD particles inside the sphere leads to an increase in the strength of the local interaction between the sphere and the fluid, as a fluid DPD particle interacts with a larger number of solid DPD particles. To address this discrepancy, we reduce the interaction parameters $a$ and $\gamma$ between a fluid DPD particle and a solid DPD particle by a factor of 27. Accordingly, $\sigma$ is reduced by a factor of $\sqrt{27}$ to satisfy the fluctuation-dissipation relationship.

B. Solid-fluid boundary conditions

The repulsive force between DPD particles is relatively weak and fluid particles may penetrate into the solids. Therefore, a reflection boundary condition is used. When a fluid particle gets into the walls, it is specularly reflected back into the fluid to the symmetric position about the inner surface of the wall. The sign of the velocity of the particle in the direction normal to the wall is also changed. In the case of the colloidal particles, when a fluid particle gets inside the solid sphere, the particle is assigned a new random velocity, corresponding to the temperature of the system, and radially moved outside of the spherical particle. Furthermore, to ensure the no-slip boundary condition at the solid-fluid interface, we artificially set the average velocity of the fluid particles close to the wall to zero. We do this for both solid walls and colloidal particles by assigning a random velocity to each fluid DPD particle that is within a thin layer next to the solid surface, $\Delta=0.05$. The random velocity assigned to the particles follows the Gaussian distribution that corresponds to the temperature of the system.
C. DPD repulsion, dissipation, and noise parameters

The thermodynamic and transport properties of the DPD fluid are determined by the choice of the repulsion \( a \), dissipation \( \gamma \), and random noise \( \sigma \) parameters. We now discuss the value of these parameters in terms of the DPD characteristic units of length \( r_c \), energy \( \varepsilon_c \), and mass \( m_c \). First, and following previous work, we choose the density of DPD particles to be \( \rho = 4 \). Therefore, for a characteristic size \( r_c \equiv 0.1 \ \mu m \), the unit of mass that would correspond to liquid water is \( m_c \equiv 2.5 \times 10^{-19} \ \text{kg} \), corresponding to \( N_m \sim 10^7 \) water molecules in a DPD particle. Next, the repulsion parameter \( a \) determines, in part, the equation of state of the DPD fluid and, in order to reproduce the dimensionless compressibility of water, we use \( a_{ij} = 75kT/\rho \),

\[
a_{ij} = 75kT/\rho, \tag{1}
\]

where \( kT \) is in \( \varepsilon_c \) units. We also need to match the dimensionless parameters that are relevant to the transport of colloidal particles in water. That is, in addition to the Reynolds and Peclet numbers, which depend on the flow conditions, there is the Schmidt number, \( Sc = \nu/D \), where \( \nu \) and \( D \) are the kinematic viscosity and the diffusivity of the fluid. \( Sc \) corresponds to the ratio of momentum to mass diffusivities and depends on the fluid properties only. Previous simulations used DPD fluids exhibiting \( Sc \sim 1 \). However, for water, and solvents in general, transport of momentum is orders of magnitude faster than mass transport, with \( Sc \sim O(10^3) \). This is particularly important if one wants to capture the hydrodynamic interactions between a suspended particle and a solid wall. First of all, it has been shown that the behavior of a DPD fluid goes from a “particle regime” at low \( Sc \) numbers, exhibiting a gaslike behavior, to a “collective regime” at high \( Sc \) numbers, in which the fluid behaves more like a liquid and collisional transport of momentum dominates over kinetic transport. In addition, some numerical studies using similar mesoscopic simulation techniques have studied the dynamics of suspended particles and shown that the expected hydrodynamic behavior is recovered only in the collective regime at large Schmidt number (see, for example, Ref. 39 for a study using multiparticle-collision dynamics). Finally, as it is discussed in Ref. 40, the separation of time scales, between the characteristic time for the diffusive motion of the suspended particle and the characteristic time for momentum transport in the fluid, which is necessary to reproduce the correct hydrodynamics, is obtained in the collective regime at relatively large Schmidt numbers. Thus, in the present work, we have increased the Schmidt number of the DPD fluid by reducing the relative kinetic energy of the DPD particles. Specifically, we use \( kT = 0.05 \), which corresponds to \( \varepsilon_c = 20 \ kT \sim 10^{-19} \ \text{J} \), assuming \( T \sim 300 \ \text{K} \). Alternative approaches to increase the Schmidt number of the fluid include using a higher fluid density, increasing the repulsion parameter, using a different dissipative function \( w^D(r_{ij}) \), and increasing the cutoff radius \( r_c \). The characteristic time scale of the simulation is then \( \tau_c \sim 0.1 \ \mu\text{s} \). Note that in standard DPD simulations we have \( kT = 1 \) and \( \Delta t = 0.05 \), which correspond to an \( \sim 20\)-fold slow down in the time integration in our simulations required in order to increase the Schmidt number. Finally, we set the strength of the random noise to \( \sigma = 3.4 \) which is consistent with previously reported values. The actual value of the viscosity and Schmidt number will be determined from single fluid simulations. We also need to define the strength of the repulsive interaction between fluid and solid DPD particles. In fact, in the most general situation, we have three parameters, one for the fluid-colloid interaction \( a_{fp} \), one for the fluid-wall interaction \( a_{fw} \), and one for the wall-colloid interaction \( a_{pw} \), which becomes relevant when a suspended particle is close to a solid wall. In the case of solid walls, which have the same density as the fluid, we also use the same repulsion value, \( a_{pw} = a_{ff} \). On the other hand, we investigated different values of the particle-fluid (and particle-wall) interactions, and we discuss the results below.

II. BULK FLUID SIMULATIONS

We first simulated the behavior of bulk fluid both to validate the DPD method and to measure the remaining transport parameters, such as the diffusion coefficient of DPD particles \( D_{DPD} \) and the fluid viscosity \( \mu \). The diffusion coefficient was measured in a bulk system with dimensions of \( 6 \times 6 \times 6 \) containing 864 DPD particles. Periodic boundary conditions were implemented in all directions. The temperature was measured during the simulations and we verified that only small deviations from the desired temperature are present in the system (temperature fluctuation is within \( 3\% \)). We obtain \( D_{DPD} = (2.6 \pm 0.3) \times 10^{-5} \) from a fit to the mean square displacement of the DPD particles as a function of time. Note that this corresponds to \( D_{DPD} \sim 1.5 \times 10^{-5} \ \text{cm}^2/\text{s} \), which is one order of magnitude smaller than the diffusivity of a single water molecule. This is due to the fact that a DPD particle does not correspond to a single molecule but to \( N_m \sim 10^7 \) water molecules.

We used similar bulk systems to measure other transport and thermodynamic properties of the fluid. First, we measured the pressure-density equation of state for the DPD fluid [see Eq. (16) in Ref. 27]. We then obtained the dimensionless compressibility of the DPD fluid and confirmed that Eq. (1) is still valid for our DPD fluid parameters \( [a, \gamma, w^D(r), r_c, \sigma, w^D(r), \text{and} \theta] \) and for our working conditions \((\rho, T)\). Then, we determined the viscosity of the DPD fluid from the velocity profile of a pressure driven Poiseuille flow between parallel walls. The DPD system consisted of 7200 particles, including 6240 fluid DPD particles confined by two parallel solid walls. Each wall contained three layers of DPD particles. The walls are perpendicular to the \( z \)-axis and the two innermost layers are located at \( z = \pm 10 \). The lengths in the \( x \) and \( y \) directions are 20 and 4, respectively. An external force \( F_E \) of magnitude 0.002 is applied in the \( x \) direction to each fluid particle. Periodic boundary conditions are used in the \( x \) and \( y \) directions. The DPD particles are initially located in a fcc solid structure of the desired density. The fluid particles are then allowed to relax to its equilibrium state first and to reach steady state flow afterward during \( 4 \times 10^5 \) time steps (~1 ms). The velocity profile is obtained from the average velocity of the fluid particles over 1000\( r_c \). The temperature of the system remains constant and uniform inside the chan-
nel during the simulations. The fluid density also remains constant and uniform inside the channel except for the usual fluid layering close to the solid walls. Then, the fluid viscosity $\mu$ was obtained from a parabolic fit to the velocity profile inside the channel, $\mu = 4.7 \pm 0.1$. The unit for viscosity is $1.4 \, 10^{-5}$ Pa s. Therefore, the viscosity of the DPD fluid corresponds to $\mu \sim 0.1$ cP. Although substantially smaller, it is orders of magnitude closer to the viscosity of water than standard DPD simulations. Similarly, the Schmidt number increases substantially, $Sc \sim 500$, which corresponds to a regime in which momentum transport is orders of magnitude faster than diffusive transport, as expected for liquids.

**IV. PARTICLE-FLUID AND PARTICLE-WALL SIMULATIONS**

In the simulation of suspended colloidal particles it is important to accurately simulate both the viscous drag on the particles, as well as their self-diffusion coefficient. In confined geometries, or in the presence of solid obstacles, it is also important that the DPD method accurately reproduces the hydrodynamic interaction of the suspended particles with the solid walls.

**A. Drag on a spherical particle**

The drag force $F$ on a spherical particle of radius $R$ moving in a stagnant fluid with a relative velocity $V$ is given by:

$$F = -C_D \pi R^2 |V|V,$$

where $C_D$ is the drag coefficient. In the limit of low Reynolds numbers ($Re = 2\rho RV/\mu$), the drag coefficient becomes $C_D = 12/Re$ and Eq. (2) reduces to the Stokes’s law, $F = 6 \pi \mu RV$. In order to measure the drag we simulated the motion of a fluid past a stationary sphere located at the center of the simulation box by applying a constant force to the fluid particles. The side of the simulation box is 16 times larger than the radius of the sphere, and periodic boundary conditions are used in all three directions. Note that although the simulation box is substantially larger than the spherical particle, spurious interactions with images of the spherical particle are still present due to the long range nature of hydrodynamic forces. We will discuss this issue in more detail at the end of this section.

We first test how sensitive the drag force is to the fluid-particle interaction parameter $a_{FP}$. Figure 1 shows the drag coefficient as a function of the Reynolds number for different values of $a_{FP}$. We compare the results with the following empirical expression, generally valid for $Re < 10^5$:

$$C_D = \frac{12}{Re} + \frac{1.865}{Re^{1/2}} - \frac{0.002415 \, Re^{1/2}}{1 + 3 \times 10^{-6} \, Re^{3/2}} + 0.245.$$  (3)

The Stokes equation is also shown in Fig. 1 and, in fact, the largest difference between the empirical formula and Stokes law in the studied range is $\sim 15\%$ at $Re=1$. We can see in Fig. 1 that, as expected, the drag coefficient $C_D$ calculated from the simulations is not sensitive to the value of the fluid-particle interactions, especially for $a_{FP} \geq 120 \, kT/\rho$.

![Figure 1](image1.png)

**FIG. 1.** Drag coefficient measured for different fluid-particle interaction parameters $a_{FP}$. The solid line corresponds to the empirical formula given in Eq. (3). The dashed line corresponds to the Stokes drag. The (large) fluctuations measured in the drag force are not shown in the plot.

A source of error in our force measurements comes from the reflection boundary condition used in the simulations which, in general, does not conserve momentum. We can estimate the magnitude of this error by comparing the force acting on the solid particle, computed as the sum of all the fluid-particle interactions, with the sum of the external force acting on the DPD fluid. These two forces are equal if the total momentum in the system is conserved. The results presented in Fig. 1 were calculated based on the total force acting on the fluid atoms, and thus accounts for the forces that would be involved in the reflection of fluid particles. The error originated from the reflection boundary condition (not shown in the figure) becomes smaller as the strength of fluid-particle interactions becomes larger. For example, the error is $(12 \pm 8)\%$ for $a_{FP} = 110 \, kT/\rho$, $(6 \pm 4)\%$ for $a_{FP} = 130 \, kT/\rho$, and $(3 \pm 2)\%$ for $a_{FP} = 200 \, kT/\rho$. This is expected since the larger the fluid-particle repulsion, the smaller the number of fluid particles penetrating the sphere. Based on the previous results we decided to use $a_{FP} = 130 \, kT/\rho$ for the fluid-particle interactions.

Next, we measured the dependence of the drag force on the asymptotic fluid velocity by varying the body force applied on the fluid particles. Figure 2(a) shows the drag on a sphere of radius $R = 1$ as a function of fluid velocity. The

![Figure 2](image2.png)

**FIG. 2.** Drag force as a function of (a) velocity and (b) particle radius. In (a), $R=1$. In (b), the velocity of the fluid ranges from 0.18 to 0.6. Open symbols correspond to the (a) velocity and (b) radius calculated using Eq. (2) in the Stokes regime. Solid symbols correspond to the same calculations but including inertia effects as described by Eq. (3).
open symbols correspond to the velocity predicted by Eq. (2) in the Stokes regime. The simulations show a linear relationship that is in relatively good agreement with the Stokes law. The agreement improves when inertia effects given by Eq. (3) are considered in calculating the velocity, as shown by the solid points. In both cases, the total force acting on the fluid is used in the calculation of the velocity. In Fig. 2(b), we show the drag force as a function of the particle radius at roughly the same Reynolds number, $Re \sim 0.9$. The open symbols correspond to the particle radius calculated with Eq. (2) in the Stokes regime. A small deviation is observed as the particle radius increases. Including inertia effects in the predicted particle radius, through Eq. (3), substantially improves the agreement between theory and DPD simulations, as shown by the solid circles in Fig. 2(b). Again, the total force acting on the DPD fluid is used in the calculations in order to account for the effects of the reflection boundary condition.

Finally, as we mentioned above, a source of error in the previous simulations is the fictitious hydrodynamic interactions between the particle and its images due to the periodic boundary conditions. In fact, the drag measurements discussed above correspond to the force acting on a representative sphere in a cubic array of spheres. In our simulations the box size is 16 times larger than the radius of the sphere and thus the corresponding volume fraction is $c \approx 10^{-3}$. Although in the limit of low Reynolds numbers the difference in the drag force measured in this configuration with respect to a bulk measurement is still around 20% for $c \approx 10^{-3}$, this difference is substantially smaller for $Re \sim 1$. In fact, in Table I we show that we cannot capture the difference between our DPD measurements and bulk predictions for concentrations lower than $c \approx 10^{-3}$.

![Image](https://via.placeholder.com/150)

**TABLE I.** Finite size effects on drag force measurements.

<table>
<thead>
<tr>
<th>Box size $\times \times \times$</th>
<th>Volume fraction</th>
<th>$R$ (average velocity)</th>
<th>$F$ (drag force)</th>
<th>$Re$</th>
<th>$F/(C_\mu pR^2V^2)$</th>
<th>Error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$12 \times 12 \times 12$</td>
<td>0.0024</td>
<td>1</td>
<td>0.213</td>
<td>20.6</td>
<td>0.36</td>
<td>0.99</td>
</tr>
<tr>
<td>$16 \times 16 \times 16$</td>
<td>0.0010</td>
<td>1</td>
<td>0.499</td>
<td>49.0</td>
<td>0.85</td>
<td>0.96</td>
</tr>
<tr>
<td>$20 \times 20 \times 20$</td>
<td>0.0005</td>
<td>1</td>
<td>0.873</td>
<td>95.835</td>
<td>1.49</td>
<td>1.02</td>
</tr>
</tbody>
</table>

The agreement improves when inertia effects given by Eq. (4) are considered in calculating the velocity, as shown by the solid circles in Fig. 2(b), in which the mobility of larger particles is smaller than predicted. In fact, using the Einstein’s relation together with the measured temperature and mobility of the particles, we obtain a better agreement for larger particles. Finally, we measured the temperature of the DPD particles and found that it is the same as the temperature of the DPD fluid with less than 1% difference.

**C. Particle-wall interactions**

We now turn to the hydrodynamic interactions between a suspended sphere and solid surfaces. In particular, we investigate the motion of particles either parallel or perpendicular to two parallel walls (see Fig. 4 for a schematic representation of the system and for a description of the notation). This is enough to test hydrodynamic interactions in the Stokes regime, in which any motion can be decomposed into its parallel and perpendicular components. In addition, in the

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In Fig. 3 we show the self-diffusion coefficient for spherical particles as a function of the particle radius $R$, with $R$ varying between 0.8 and 3.0 ($80 \text{ nm}<R<300 \text{ nm}$). The diffusion coefficient obtained from the DPD simulations is in good agreement with the Stokes–Einstein relation given by Eq. (4) particularly for $R<2$. On the other hand, for larger particles the diffusivity is smaller than expected according to Eq. (4). This is consistent with the results shown in Fig. 2(b), in which the mobility of larger particles is smaller than predicted. In fact, the Einstein’s relation together with the measured temperature and mobility of the particles, we obtain a better agreement for larger particles. Finally, we measured the temperature of the DPD particles and found that it is the same as the temperature of the DPD fluid with less than 1% difference.

**B. Self-diffusion coefficient**

We measure the self-diffusion coefficient of colloidal particles suspended in bulk DPD fluid using the same simulation box as described in Sec. IV A. In this case, however, the spheres are freely suspended and we track their Brownian motion as a function of time. The translational and rotational motions of the spherical particles are integrated from the linear and angular equations of motion, following the approach presented in Ref. 31. The diffusion is then obtained from a linear fit to the mean square displacement of the colloidal particles as a function of time. For a spherical particle the self-diffusion coefficient is given by the Stokes–Einstein relation, 

$$D_p = \frac{kT}{\zeta} = \frac{kT}{6\pi\mu R^2},$$

where the first equality is the Einstein’s relation and $\zeta^{-1}$ is the mobility of the particle.

In Fig. 3 we show the self-diffusion coefficient for spherical particles as a function of the particle radius $R$, with $R$ varying between 0.8 and 3.0 ($80 \text{ nm}<R<300 \text{ nm}$). The diffusion coefficient obtained from the DPD simulations is in good agreement with the Stokes–Einstein relation given by Eq. (4) particularly for $R<2$. On the other hand, for larger particles the diffusivity is smaller than expected according to Eq. (4). This is consistent with the results shown in Fig. 2(b), in which the mobility of larger particles is smaller than predicted. In fact, using the Einstein’s relation together with the measured temperature and mobility of the particles, we obtain a better agreement for larger particles. Finally, we measured the temperature of the DPD particles and found that it is the same as the temperature of the DPD fluid with less than 1% difference.

![Image](https://via.placeholder.com/150)

**FIG. 3.** Diffusion coefficient as a function of particle size. Solid circles correspond to the measured diffusion coefficient. Open circles correspond to the diffusion coefficient corrected by the mobility of the spheres (see text).
Stokes regime, the hydrodynamic force in this system depends only on two dimensionless parameters, for example, $h/R$ and $h/d$ (see Fig. 4). In all cases a small constant force $F_E$ is applied to the spherical particle, and the corresponding Reynolds numbers are relatively small, $Re<0.1$, especially for close particle-wall separations. The drag force acting on the particle is larger than the Stokes force due to the presence of the solid walls, and it is usual to write it in terms of a correction factor $\lambda$.

$$ F = 6\pi\mu R\lambda V. \quad (5) $$

We first consider the drag force acting on a spherical particle moving parallel to the walls. The distance from the center of the sphere to the upper wall is three times the distance from the lower wall. That is, we are going to vary $h/R$ and the other parameter is determined by the previous condition. Given the asymmetric position of the particle with respect to the walls [see Fig. 4(a)], the solid sphere rotates with but a small angular velocity.\(^{(48)}\) In the simulations, the particles are free to rotate and the correction factor $\lambda$ is measured for different particle-wall interaction parameters $a_{PW}$. After a relaxation time of $3 \times 10^4$ steps, the sphere moves with the constant average velocity at which the external force is balanced by the drag. (Note that the largest characteristic time for momentum diffusion, $4L^2/\nu=400$ for $L=10$, is almost two orders of magnitude smaller than the relaxation time.) We then measure the correction factor $\lambda$ for different relative separations by changing either $R$ or $h$, ranging from $R=1$ and $h=9$ for the largest relative separation to $R=2.1$ and $h=0.1$ for the smallest particle-wall gap. The results of four independent simulations are used to obtain the average drag on the particle for each particle-wall separation.

For large separations, $h/R \gg 1$, the wall effect vanishes and we should recover Stokes law, $\lambda=1$. However, hydrodynamic interactions are long ranged, and for $h/R \sim 10$ the predicted correction is still relatively large, $\sim 7\%$.\(^{(49)}\) Therefore, in Fig. 5 we compare the simulation results with theoretical predictions for the correction factor $\lambda$ over a wide range of separations, with $0.04<h/R<10$. The simulation results are in excellent agreement with the analytical results for the entire separation range. It is noted that the observed agreement with continuum results was not expected for particle-wall separations comparable to the size of the DPD fluid particles when the number of fluid particles in the gap between the sphere and the wall becomes small. For example, the average number of DPD fluid particles between the sphere and the wall and within a cylinder with the same radius as the sphere is $O(100)$ for $R=3$ and $h=0.3$, but $O(10)$ for $R=2$ and $h=0.2$, and $O(1)$ for $R=1$ and $h=0.1$. Let us note that similarly surprising results concerning the robustness of continuum calculations have been also observed in molecular dynamics simulations.\(^{(50-53)}\) In addition, in the DPD simulations, the interactions between a solid DPD particle and a DPD particle in the moving sphere include a dissipative force that is proportional to the relative velocity between them and, therefore, contributes to the drag force.

We also present results corresponding to different values of the particle-wall interaction parameter $a_{PW}$. We can see that, as expected, the strength of the particle-wall interaction $a_{PW}$ does not affect the drag force on the particles moving parallel to the walls. Moreover, at distances larger than the cutoff $r_c$ the magnitude of the particle-wall interaction is clearly irrelevant. On the other hand, the net effect of these forces will resist the particle from getting close to the wall and thus $a_{PW}$ will affect the motion perpendicular to the walls.

Next, we consider the drag on a spherical particle moving toward one of the walls, as shown in Fig. 4(b). In this case, the geometry of the system is determined by $2R/d$ and the remaining parameter, such as $h/R$, varies as the particle moves. To compare with theoretical predictions we consider two cases: $d/2R=3$ and $d/2R=5$. For each case, we study two different systems: One with $R=1$ and one with $R=2$. In the simulations, particles are free to rotate and move from well above the midplane between the walls toward the lower wall under a small, constant external force. The drag force and velocity are only measured after the particles cross the midplane between the walls, and we assume that the system has reached equilibrium. We performed 200 (100) different realizations of the simulations with $R=1$ ($R=2$) to obtain a relatively accurate average velocity at each separation $h$. Figure 6 shows the correction factor $\lambda$ as a function of the relative distance between the sphere and the wall, $h/R$. The results are in good agreement with numerical solutions obtained by Ganatos et al.\(^{(55)}\) for both $d/2R=3$ and $d/2R=5$. The case $R=2$ slightly overestimates the value of the drag correction factor for $d/2R=5$ and $h/R>1$. The difference between the theory and the simulations in this case is $\sim 10\%$.

Let us note that, as in the case of parallel motion, the force on the moving sphere has two different contributions: (i) Particle-wall conservative and dissipative forces and (ii)
 particle-fluid interactions. In Fig. 6(a) we also present the purely hydrodynamic interaction, originating from particle-fluid interactions only. This contribution deviates from the continuum prediction when separations are comparable to the size of the DPD fluid particles. In fact, we can see that both $R=1$ and $R=2$ results deviate from the continuum predictions at a similar absolute separation, $h=0.6$. As a consequence, the larger sphere is able to reproduce the hydrodynamic interaction down to smaller relative separations, $h/R \sim 0.3$.

In the final set of simulations we investigate the motion of a spherical particle inside a cylindrical tube. In fact, we will compare the results with numerical solutions obtained for an infinite row of rigid spheres moving in a viscous fluid. This allows us to compare the measured particle-wall hydrodynamic interactions with exact solutions. That is, the periodic boundary conditions used in our simulation mimic the system exactly. In Fig. 7 we show the results of the correction factor to the Stokes law, $\lambda$, as a function of $D/2R$, where $D$ is the diameter of the cylinder. For $D/2R \gg 1$, the DPD results are in good agreement with the numerical solutions. More important, the agreement improves for larger particles with an error of $\sim 10\%$ for $D/2R > 2.5$. For even smaller clearances we observe large deviations possibly due to the reduction in the number of fluid particles in the gap between the suspended particle and the tube wall and the increased relative roughness of the tube walls as the diameter is reduced.

V. SUMMARY

We have investigated the use of DPD to model the transport of colloidal particles in bulk and in confined geometries with special focus on the hydrodynamic interactions between a suspended particle and a solid wall. First, we determine the appropriate parameters in the DPD simulations that result in a relatively large Schmidt number, $Sc \gg 1$, something that is important in the simulation of colloidal particles in confined geometries. We achieve this by increasing the ratio between the strength of the dissipative force and the kinetic energy of the DPD particles. We then measured particle-fluid interactions and found good agreement with theoretical predictions for both the drag force and the diffusion coefficient. We then focused on the particle-solid interactions. We measured the force on a colloidal particle moving both parallel and perpendicular to two parallel planes. In both cases we found good agreement with the theoretical predictions based on Stokes flows. It is important to note that we observe good agreement for particle-wall separations as small as $0.1R$, and for particles as small as $R=1$. Finally, we also tested the DPD method using periodic solutions. In this case, we measured the drag on a line of spheres moving through a cylindrical tube for different ratios between the particle and tube radii, and found good agreement with the continuum results.


