

A Spring Model for Suspended Particles in Dissipative Particle Dynamics

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Abstract This paper is concerned with the use of oscillating particles instead of the usual frozen particles to model a suspended particle in the Dissipative Particle Dynamics (DPD) method. A suspended particle is represented by a set of basic DPD particles connected to reference sites by linear springs of very large stiffness. The reference sites, collectively modelling a rigid body, move as a rigid body motion calculated through their Newton-Euler equations, using data from the previous time step, while the velocities of their associated DPD particles are found by solving the DPD equations at the current time step. In this way, a specified Boltzmann temperature (specific kinetic energy of the particles) can be maintained throughout the computational domain, including the region occupied by the suspended particles. This parameter can also be used to adjust the size of the suspended and solvent particles, which in turn affect the strength of the shear-thinning behaviour and the effective maximal packing fraction. Furthermore, the suspension, comprised of suspended particles in a set of solvent particles all interacting under a quadratic soft repulsive potential, can be simulated using a relatively large time step. Several numerical examples are presented to demonstrate attractiveness of the proposed model.

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1 Introduction

Dissipative Particle Dynamics (DPD), originally proposed by Hoogerbrugge and Koelman (1992) as a mesoscopic simulation technique for a complex fluid, has received considerable attention in the last two decades. Its formulation is derived from the view that each DPD particle is a coarse-grained representation of a group of fluid particles. DPD particles interact through a soft potential and thus the simulation can be carried out on length and time scales far beyond those associated with Molecular Dynamics (MD). Viscous interactions are accounted for by dissipative forces depending on the relative velocity of the particle. It is important to note that ensemble-average quantities formed from the DPD particle states (positions and velocities) satisfy the conservation of mass and momentum [Español (1995)], and thus the method is qualified as a particle-based method for solving continuum problems. One of the most attractive features of DPD is that its ability to model complex fluids in a simple way. A subset of DPD particles can be constrained to form a solid object [Koelman and Hoogerbrugge (1993)], a droplet [Clark et al. (2000)], a polymer chain [Kong et al. (1997)], etc. DPD method has been used with varying degree of success in simulating various classes of complex fluids, for examples, colloidal suspensions [Koelman and Hoogerbrugge (1993); Boek et al. (1997); Chen et al. (2006); Pan et al. (2010a)], fluid mixtures [Novik and Coveney (1997); Laradji and Hore (2004)], polymer solutions [Kong et al. (1997); Jiang et al. (2007)], polymer melts [Nikunen et al. (2007)], and red blood cell modelling [Pan et al. (2010b), Ye et al. (2013)] - this list is not meant to be exhaustive. We noted some recent efforts in the development of a thermodynamically consistent DPD model, where two addition variables, the particle volume and the internal energy, were introduced, and its applications explored [Español and Revenga (2003); Bian et al. (2012); Kulkarni et al. (2013); Gatsonis et al. (2014)].

This study is mainly concerned with a new DPD model for particulate suspensions, and its applications in a few flow problems of interest. In the DPD method, a suspended particle can be modelled using frozen DPD particles [Koelman and Hoogerbrugge (1993); Boek et al. (1997);

Martys (2005); Chen et al. (2006)], or just using a single DPD particle [Dzwinel and Yuen (2000); Pryamitsyn and Ganesan (2005); Pan et al. (2008); Pan et al. (2010a); Whittle and Travis (2010); Groot (2012); Mai-Duy et al. (2013)]. Each type of model has its own strengths and weaknesses.

In the single-particle models, a single DPD particle is used to represent a suspended particle, referred here as the colloidal particle (C); its velocity and position are updated according to its DPD equations. The solvent is represented by a set of DPD particles, referred to as solvent particles (S). Between them, there are three types of interactions: solvent-solvent (SS), solvent-colloidal (SC), and colloidal-colloidal (CC) interactions. In [Pan et al. (2010a)], for SC and CC interactions, the conservative force is taken as a steep exponential potential. Such a steep form for the conservative force was deemed necessary to produce a uniform colloidal dispersion [Pan et al. (2010a)]. Stokes results are then utilised to determine the strength of the dissipative forces. In [Mai-Duy et al. (2013)], the mass of DPD particles is allowed to approach zero to induce a nearly incompressible slow viscous flow in a DPD fluid and to enhance its dynamic response. In [Dzwinl and Yuen (2000) and Pryamitsyn and Ganesan (2005)], the CC and CS interactions are implemented with the energy conserving Lennard-Jones (L-J) two-body potentials. The main advantage of single-particle models is that only a one DPD particle is required to model a suspended particle. However, these models are limited to spherical (3D) and circular (2D) suspended particles only, and require more effort in the process of determining the DPD parameters, particularly when the suspended particles are polydispersed in sizes. Furthermore, the use of L-J potentials and exponential conservative forces, rather than soft potentials (linear forces), places some restriction on the time step, increasing the computational effort. Also, a linked-list algorithm needs be modified for an efficient computation as interaction zones are of different sizes [Pryamitsyn and Ganesan (2005)].

The frozen-particle model consists in employing a subset of the same DPD particles, which remain at a fixed relative position, to represent a suspended particle. Its velocity and position are updated using the sums of forces and torques acting on it. The model has the ability to represent a suspended particle of arbitrary shape and size, defined by the configuration of its constituent particles. Since the constituent particles are frozen, the dissipative forces between themselves vanish and a specified constant temperature (specific kinetic energy) may not be easily maintained throughout the simulation domain, for a finite small time step. In practice, a large number of

basic DPD particles are employed (a few hundreds) to model a spherical particle [Martys (2005); Chen et al. (2006)] and thus the computational effort is much higher than that for single-particle models.

In this study, we propose a simple but effective DPD model to alleviate some of the weaknesses of single particle models (small time steps, complex interactions, spherical/cylindrical shape limitations), and the frozen particle models (large systems, difficulty in maintaining the system temperature), and also address some implementation issues concerning the number density and the volume fraction in DPD. Here, a suspended particle is modelled using a few basic DPD particles (“constituent particles”) that are tethered to reference sites on a surface, and fully interact with each other and with the rest of the DPD system. It will be shown that the size of a colloidal particle is decided by the repulsion acquired from the superimposition of conservative forces of constituent particles of the colloidal particle (not by the reference sites). This allows a circular/spherical shape for a suspended particle to be achieved with a few basic DPD particles only. In this study, a hard disc (2D circular cylinder), or a spherical suspended particle can be modelled by 4 or 8 basic DPD particles, respectively. The constituent particles of a colloidal particle are connected to the reference sites via linear springs of large stiffness. This allows a specified temperature to be maintained over the entire domain inclusively. This parameter has been shown to influence the fluid compressibility [Marsh (1998)]; it is shown here that it also controls some physical characteristics of the suspension, such as the strength of its shear-thinning behaviour and/or the effective size of the solvent and colloidal particles. The other computational advantage of the proposed model is that all the DPD parameters are the same as those representing the solvent. This implies (i) there is no need to perform a numerical parametrisation study for the interactions between solvent and colloidal particles; (ii) the underlying particles all interact through a soft potential (linear forces) and thus allowing large time steps in the suspension simulation; and (iii) all interactions between particles can use the same cutoff radius and therefore allow one to use a simple, single level linked-list algorithm.

At highly concentrated regime, short-range lubrication forces are expected to be dominant, and can only be mimicked if the presence of the solvent between colloid particles can still be maintained. Only standard DPD forces, namely conservative, dissipative and random forces, are employed;

no approximate lubrication approximation is used unlike some other particle-based methods (e.g., SPH, or sDPD). The number density, fluid velocities and stresses in DPD are calculated by averaging the instant results (particle configuration, particle velocities, etc.) over very large numbers of time steps.

The remainder of the paper is organised as follows. Section 2 provides a brief overview of the standard DPD equations. The proposed spring model for suspended particles is described in Section 3 and then verified numerically in Section 4. Section 5 gives some concluding remarks.

2 Dissipative Particle Dynamics

Governing equations:

The stochastic differential equations governing the motion of a DPD particle are given by

$$\dot{\mathbf{r}}_i = \mathbf{v}_i, \tag{1}$$

$$m_i \dot{\mathbf{v}}_i = \mathbf{F}_i, \tag{2}$$

where m_i , \mathbf{r}_i and \mathbf{v}_i represent the mass, position and velocity vectors of a particle $i = 1, \dots, N$, respectively, N is the total number of DPD particles, the superposed dot denotes a time derivative, and \mathbf{F}_i is the total force vector exerted on particle i , containing three parts

$$\mathbf{F}_i = \sum_{j=1, j \neq i}^N (\mathbf{F}_{ij,C} + \mathbf{F}_{ij,D} + \mathbf{F}_{ij,R}), \tag{3}$$

in which the sum runs over all other particles except i , within a certain cutoff radius r_c . Outside the cutoff radius (which is the same for $\mathbf{F}_{ij,D}$ and $\mathbf{F}_{ij,R}$ but may be different for $\mathbf{F}_{ij,C}$), these forces are set to zero. The first term on the right is referred to as conservative force (subscript C), the second, dissipative force (subscript D) and the third, random force (subscript R). The three forces

are pairwise and are usually given in the forms

$$\mathbf{F}_{ij,C} = a_{ij}w_C\mathbf{e}_{ij}, \quad (4)$$

$$\mathbf{F}_{ij,D} = -\gamma w_D (\mathbf{e}_{ij} \cdot \mathbf{v}_{ij}) \mathbf{e}_{ij}, \quad (5)$$

$$\mathbf{F}_{ij,R} = \sigma w_R \theta_{ij} \mathbf{e}_{ij}, \quad (6)$$

where a_{ij} , γ and σ are constants reflecting the strengths of these forces, w_C , w_D and w_R the configuration-dependent weighting functions to be defined below, $\mathbf{e}_{ij} = \mathbf{r}_{ij}/r_{ij}$ a unit vector from particle j to particle i ($\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$, $r_{ij} = |\mathbf{r}_{ij}|$), $\mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j$ the relative velocity vector, and θ_{ij} a Gaussian white noise ($\theta_{ij} = \theta_{ji}$) with stochastic properties

$$\langle \theta_{ij} \rangle = 0, \quad (7)$$

$$\langle \theta_{ij}(t)\theta_{kl}(t') \rangle = (\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \delta(t - t'), \quad (8)$$

with $\delta(t - t')$ the Dirac delta function, and δ_{ij} the Kronecker delta.

It was shown in [Español and Warren (1995)] that the followings

$$w_D(r_{ij}) = (w_R(r_{ij}))^2, \quad (9)$$

$$k_B T = \frac{\sigma^2}{2\gamma}, \quad (10)$$

lead to a detailed balance of the system (equi-partition principle or fluctuation-dissipation theorem). This relates the strength of the dissipative force to the strength of the random force through the definition of the thermodynamic temperature (constant fluctuation kinetic energy). A popular choice of the weighting functions is [Groot and Warren (1997); Fan et al. (2006)]

$$w_C(r_{ij}) = 1 - \frac{r_{ij}}{r_c}, \quad (11)$$

$$w_D(r_{ij}) = \left(1 - \frac{r_{ij}}{r_c}\right)^s. \quad (12)$$

where s is a constant ($s = 2$ and $s = 1/2$ are two typical values of s).

We may re-write the stochastic DPD equation (2) in the following differential form

$$\Delta \mathbf{v}_i = \frac{1}{m_i} \sum_{j \neq i} a_{ij} w_C \Delta t \mathbf{e}_{ij} - \frac{1}{m_i} \sum_{j \neq i} \gamma w_D (\mathbf{e}_{ij} \cdot \mathbf{v}_{ij}) \Delta t \mathbf{e}_{ij} + \frac{1}{m_i} \sum_{j \neq i} \sigma w_R \Delta W_{ij}(t, \Delta t) \mathbf{e}_{ij}, \quad (13)$$

where

$$\Delta W_{ij}(t, \Delta t) = \int_t^{t+\Delta t} \theta_{ij}(s) ds. \quad (14)$$

The incremental stochastic process ΔW_{ij} has zero mean and autocorrelation

$$\langle \Delta W_{ij}(\Delta t) \Delta W_{kl}(\Delta t) \rangle = (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) \Delta t. \quad (15)$$

If we define $\Delta W_{ij} = \xi_{ij} \sqrt{\Delta t}$, then ξ_{ij} is a Gaussian random tensor with zero mean and variance $\langle \xi_{ij} \xi_{kl} \rangle = (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk})$. This random tensor can be chosen from a pseudo-random sequence, and (13) is the basis for updating a particle velocity. Since w_C , w_D and w_R are dimensionless functions, the DPD parameters a_{ij} , γ , σ and $k_B T$ have units of $[F]$, $[FT/L]$, $[F\sqrt{T}]$ and $[FL]$, respectively, where $[F]$ is the force unit, $[T]$ is the unit of time, $[L]$ is the unit of length.

Calculation of Stress Tensor:

The flow domain is divided into grids and local field data are collected in each bin. The flow properties are calculated by time averaging over all sampled data in each bin. The stress tensor is calculated using the Irving-Kirkwood expression [Irving and Kirkwood (1950)]

$$\mathbf{S} = -\frac{1}{V} \left[\sum_i m \mathbf{V}_i \mathbf{V}_i + \frac{1}{2} \sum_i \sum_{j \neq i} \mathbf{r}_{ij} \mathbf{F}_{ij} \right] = -n \left(\langle m \mathbf{V} \mathbf{V} \rangle + \frac{1}{2} \langle \mathbf{r} \mathbf{F} \rangle \right), \quad (16)$$

where n is the number density of particles, V is the volume of the bin and \mathbf{V}_i is the velocity fluctuation of particle i with respect to the mean field velocity (peculiar velocity). The first term on the right side of (16) denotes the contribution to the stress from the momentum (kinetic) transfer of DPD particles and the second term from the interparticle forces. The constitutive pressure can be determined from the trace of the stress tensor:

$$p = -\frac{1}{3} \text{tr} \mathbf{S}. \quad (17)$$

Time scales in particulate suspensions:

In the micromechanics as represented by Eq. (2), there are three time scales: the smallest fluctuation time scale of the random forces, the inertial time scale formed by mass and dissipative forces ($m\gamma^{-1}$), and the relaxation time scale, formed by the dissipative and conservative forces ($\gamma a_{ij}^{-1} r_c$).

In assessing the global behaviour of a colloidal suspension, one tends to concentrate on two relevant time scales: (i) the diffusion time scale that restores the equilibrium configuration: a^2/D_0 (a is the sphere radius and D_0 the single-sphere diffusion coefficient); and (ii) the time scale on which the structure of the dispersion is deformed by the shear: $\dot{\gamma}^{-1}$ ($\dot{\gamma}$ the shear rate). The Péclet number is defined as the ratio between the two time scales

$$Pe = \dot{\gamma} a^2 / D_0. \quad (18)$$

This dimensionless shear rate is a measure of the relative importance of dissipative (hydrodynamic contribution) and diffusion (random contribution) forces.

Conservation properties:

From the system state (positions and velocities of DPD particles), one can define the local fluid density:

$$\rho(\mathbf{r}, t) = \left\langle \sum_i m \delta(\mathbf{r} - \mathbf{r}_i) \right\rangle = mn(\mathbf{r}, t), \quad (19)$$

where $n(\mathbf{r}, t)$ is the number density, and the local linear momentum:

$$\rho(\mathbf{r}, t) \mathbf{u}(\mathbf{r}, t) = \left\langle \sum_j m \mathbf{v}_j \delta(\mathbf{r} - \mathbf{r}_j) \right\rangle. \quad (20)$$

These quantities so defined have been shown to satisfy conservation laws [Español (1995); Marsh et al. (1997)]:

$$\frac{\partial}{\partial t} \rho(\mathbf{r}, t) + \nabla \cdot (\rho(\mathbf{r}, t) \mathbf{u}(\mathbf{r}, t)) = 0, \quad \nabla = \partial / \partial \mathbf{r}, \quad (21)$$

and

$$\frac{\partial}{\partial t} (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = \nabla \cdot \mathbf{S}. \quad (22)$$

Thus, DPD may be regarded as a particle-based method for solving continuum flow problems (21)-(22) - in some physical sense it is a particle discretisation of (21)-(22). In this particle-based point of view, then DPD particles may be thought of as a model of a behaviour (e.g., viscous compressible fluid), not merely a cluster of fluid particles. Phenomena in the length scale below a particle length scale are ignored by the method. The complex nature of the fluid is described in its microstructure, for example, a standard set of DPD particles under dissipative and random interaction forces have been shown to be a compressible Newtonian fluid [Marsh (1998)], a suspension of dumbbell particles (constructed by chaining two DPD particles by linear springs) behaves like an Oldroyd-B fluid [Phan-Thien, 2013].

3 Proposed model for suspended particles

It was reported in Sierou and Brady (2001) that in Stokesian Dynamics simulation a system with larger number of particles tends to capture more accurately the properties of suspensions than one with fewer particles. Our strategy in this work is also to maximize the number of suspended particles. To accomplish this goal, we propose to model a suspended particle by a set of p basic DPD particles (p is small) connected to reference sites by linear springs. For example, as shown in Figure 1, a hard disc may be simply constructed using 3 or 4 basic DPD particles, whose associated reference sites are located at the vertices of an equilateral triangle or square. A spherical particle may be represented using 6 or 8 basic DPD particles with their reference sites at the vertices of either an octahedron or a cube. The schematic diagram for the case of a suspended disc using 4 basic DPD particles is illustrated in Figure 2. The reference sites are updated according to their Newton-Euler equations, subjected to the constraint

$$\xi_{ij}(t) \equiv (\bar{\mathbf{r}}_i(t) - \bar{\mathbf{r}}_j(t))^T (\bar{\mathbf{r}}_i(t) - \bar{\mathbf{r}}_j(t)) - (d_{ij})^2 = 0, \quad (23)$$

where d_{ij} is the fixed distance between the sites i and j , and $\bar{\mathbf{r}}_i$ the position of the reference site i (the overline is used to differentiate the site from its associated DPD particle). This model allows the constituent particles of a colloidal particle to be treated in the same manner as the solvent particles (i.e., subject to the same DPD parameters including $k_B T$), from which one can control

the effects of $k_B T$ on the flow properties in a systematic way, leading to a good definition of the volume fraction through the number of basic DPD particles.

Consider the k th suspended particle, comprised of a set of p basic DPD particles and their associated reference sites. Its mass centre is located at

$$\mathbf{R}_c^k = \frac{1}{M_c^k} \left(\sum_{i=1}^p m_i^k \mathbf{r}_i^k + \sum_{i=1}^p \bar{m}_i^k \bar{\mathbf{r}}_i^k \right), \quad M_c^k = \sum_{i=1}^p m_i^k + \sum_{i=1}^p \bar{m}_i^k, \quad (24)$$

where M_c^k is its total mass. Its base, formed by a set of reference sites, is assumed to move as a rigid body according to its Newton-Euler equations, with negligible mass ($\bar{m}_i^k \rightarrow 0$). At very large spring stiffness, $\mathbf{r}_i^k(t) \rightarrow \bar{\mathbf{r}}_i^k(t)$, its centre of mass can be approximately taken to be the centre of its constituent particles

$$\mathbf{R}_c^k \approx \frac{1}{M_c^k} \left(\sum_{i=1}^p m_i^k \mathbf{r}_i^k \right) \approx \frac{1}{M_c^k} \left(\sum_{i=1}^p m_i^k \bar{\mathbf{r}}_i^k \right), \quad M_c^k \approx \sum_{i=1}^p m_i^k. \quad (25)$$

The force on a constituent particle of the k th suspended particle is

$$\mathbf{F}_i^k(t) = \sum_{j=1, j \neq i}^N [\mathbf{F}_{ij,C}^k(t) + \mathbf{F}_{ij,D}^k(t) + \mathbf{F}_{ij,R}^k(t)] + \mathbf{F}_{i,S}^k(t), \quad i = (1, 2, \dots, p). \quad (26)$$

where $\mathbf{F}_{i,S}^k(t) = -H [\mathbf{r}_i^k(t) - \bar{\mathbf{r}}_i^k(t)]$ is the spring force with H being the stiffness of the spring.

The force on a reference site of the k th suspended particle is

$$\bar{\mathbf{F}}_i^k(t) = \bar{\mathbf{F}}_{i,S}^k(t) + \mathbf{G}_i^k(t), \quad i = (1, 2, \dots, p), \quad (27)$$

where $\bar{\mathbf{F}}_{i,S}^k$ and \mathbf{G}_i^k are the spring and constraint forces, respectively. The latter is given by

$$\mathbf{G}_i^k(t) = - \sum_{j=1}^p \lambda_{ij}(t) \nabla_i \xi_{ij}(t), \quad (28)$$

where $\lambda_{ij}(t)$ are the time-dependent Lagrange multipliers and ∇ is the gradient with respect to the coordinates of the reference site under consideration. Note that $\lambda_{ij}(t) = \lambda_{ji}(t)$, $\xi_{ij}(t) = \xi_{ji}(t)$ and $\nabla_i \xi_{ij}(t) = -\nabla_j \xi_{ij}(t)$.

Using (26) and (27), the net force and torque on the k th colloidal particle are expressed as

$$\mathbf{F}^k = \sum_{i=1}^p \mathbf{F}_i^k(t) + \sum_{i=1}^p \bar{\mathbf{F}}_i^k(t), \quad (29)$$

$$\mathbf{T}^k = \sum_{i=1}^p (\mathbf{r}_i^k - \mathbf{R}_c^k) \times \mathbf{F}_i^k(t) + \sum_{i=1}^p (\bar{\mathbf{r}}_i^k - \mathbf{R}_c^k) \times \bar{\mathbf{F}}_i^k(t). \quad (30)$$

Since the constraint forces and the spring forces are pairwise, expressions (29) and (30) reduce to

$$\mathbf{F}^k = \sum_{i=1}^p \sum_{j=1, j \neq i}^N [\mathbf{F}_{ij,C}^k(t) + \mathbf{F}_{ij,D}^k(t) + \mathbf{F}_{ij,R}^k(t)], \quad (31)$$

$$\mathbf{T}^k = \sum_{i=1}^p (\mathbf{r}_i^k - \mathbf{R}_c^k) \times \sum_{j=1, j \neq i}^N [\mathbf{F}_{ij,C}^k(t) + \mathbf{F}_{ij,D}^k(t) + \mathbf{F}_{ij,R}^k(t)]. \quad (32)$$

Note that the sum of the spring forces on the constituent particles are absent in the net force and torque on the colloidal particle.

The velocity of the mass centre and the angular velocity of the k th colloidal particle are obtained from its Newton-Euler equations:

$$M_c^k \frac{d\mathbf{V}_c^k}{dt} = \mathbf{F}^k(t), \quad (33)$$

$$\mathbf{I}^k \frac{d\boldsymbol{\omega}^k}{dt} = \mathbf{T}^k(t) + \boldsymbol{\omega}^k \times (\mathbf{I}^k \boldsymbol{\omega}^k), \quad (34)$$

where \mathbf{I}^k is the moment of inertia tensor of the colloidal particle, and its reference sites are advanced according to

$$\frac{d\bar{\mathbf{r}}_i^k}{dt} = \mathbf{V}_c^k + \boldsymbol{\omega}^k \times (\bar{\mathbf{r}}_i^k - \mathbf{R}_c^k), \quad i = (1, 2, \dots, p), \quad (35)$$

while the corresponding velocities of the constituent particles are to be found from solving equation $m_i \dot{\mathbf{v}}_i^k = \mathbf{F}_i^k$, $i = (1, 2, \dots, p)$, with \mathbf{F}_i^k given in (26).

It can be seen from our model that there is only one type DPD particles, and therefore one set of DPD parameters, a feature to be contrasted with the single-particle models. On the other hand, since the constituent particles undergo relative oscillatory motions about their associated reference sites, there are dissipative forces between them, a feature to be contrasted to the frozen-particle models. We will next report numerical results to support the proposed model.

4 Numerical examples

The proposed model will be tested in Couette and Poiseuille flows. The simulation is carried out on a domain of 10×10 and 20×20 for 2D, and $20 \times 10 \times 20$ for 3D with the following DPD parameters: $m_i = 1$, $s = 1/2$, $n = 4$, $a_{ij} = 18.75$, $\sigma = 3$ and $r_c = 1$. Springs associated with the constituent particles should be stiff in order to represent a rigid body correctly. In the present calculations, the stiffness of springs is chosen to be quite large (i.e., $H = 3000$ after some experimentations) to model a solid body, allowing the constituent particles to fully participate in the system dynamics, leading to a better control of the system temperature. Results concerning spring forces are normalised with $a_{ij} = 18.75$ (the maximum conservative force), the effective viscosity of the suspension is normalised with the viscosity of the suspending fluid, and the normal stress difference with the product of the solvent viscosity and the shear rate. The improvement of the proposed model, particularly in time step and simplicity over the single particle model, and in the system size and temperature variation over the frozen particle model will be demonstrated.

4.1 Shapes of colloidal particles

In frozen particle models, DPD particles are arranged in layers on the suspended particle to achieve a desired shape - these particles move in a rigid body motion and do not participate in the DPD dynamics. The radius of the colloidal particle is defined as the distance from the centre of the sphere to the centre of a frozen particle located on the surface for a spherical suspended particle [Chen et al. (2006)]. As a result, a large number of constituent particles is normally required. For example, in [Chen et al. (2006)], at least 500 particles per sphere were used. In our model, only a few DPD particles (per suspended particle) are required, and we observe here that the repulsion resulting from the superimposition of shape functions for the conservative forces of the constituent particles actually account for the shape of the colloidal particle. To have a conical shape with a flat round base, one may need to employ a few constituent particles only. It is possible to use 3 or 4 basic DPD particles to represent a 2D circular disc, and 6 or 8 DPD particles for a spherical particle (Figure 1). A condition required here for an axisymmetric suspended particle is that its reference sites should be located axisymmetrically. Consider a 2D circular disc. Figure 3 shows the contours of the

superimposition of the conservative forces on all the constituent particles, i.e., $\sum_{i=1}^p a_{ij}(1 - r_{ij}/r_c)$, for two simple cases, $p = 3$ and $p = 4$. Figure 4 shows contour plots of the radial component of the total conservative force vector on a suspended particle, i.e., $\sum_{i=1}^p a_{ij}(1 - r_{ij}/r_c)\mathbf{e}_{ij} \cdot \mathbf{e}_{oj}$ (o the centre of the suspended particle). In both cases a conical-like repulsion shape can be obtained. In the following simulations, we will employ 4 basic DPD particles to represent a 2D circular disc and 8 basic DPD particles for a spherical particle. The distance between the two nearest reference sites should be chosen not too large; otherwise, solvent particles can easily penetrate the core region. Increasing this distance increases the size of the particle; however, after some investigation, this distance is taken as 0.25 DPD units. Larger suspended particles may be modelled conveniently with more constituent particles, keeping the distance between neighbouring pairs about 0.25 DPD units.

4.2 Number density

The approximate analysis of Marsh et al. (1997), based on no conservative force ($a_{ij} = 0$), yields the following results

$$\eta = \frac{15mk_B T}{8\pi\gamma r_c^2} + \frac{4\pi\gamma n^2 r_c^4}{315} \text{ (for 2D)}, \quad \eta = \frac{315mk_B T}{128\pi\gamma r_c^3} + \frac{512\pi\gamma n^2 r_c^5}{51975} \text{ (for 3D)}, \quad (36)$$

for the viscosity, and

$$D = \frac{15k_B T}{4\pi n\gamma r_c^2} \text{ (for 2D)}, \quad D = \frac{315k_B T}{64\pi n\gamma r_c^3} \text{ (for 3D)}, \quad (37)$$

for the self-diffusion coefficient. These physical quantities are functions of mass, number density, cut-off radius, temperature and strength of the dissipative force. In suspension simulations, the DPD parameters for the solvent should yield the same values for the pure solvent physical parameters, including its viscosity, density. It is straightforward to meet such a requirement for the DPD parameters other than the number density. There have been different reports on how to handle the solvent number density: (i) as the suspended particles are introduced, the number of solvent particles are reduced to keep the number density of the whole system the same as that of

the solvent (e.g., [Jamali et al. (2013)]); and (ii) the solvent density is defined conventionally as $n_S = N_S/(V - V_C)$, where N_S is the number of solvent particles, V the volume of the simulation box (total volume) and V_C the volume of the colloidal particles (e.g., [Whittle and Travis (2010); Groot (2012)]).

The two approaches just mentioned will cause the solvent number density, defined as

$$n(\mathbf{r}, t) = \left\langle \sum_i \delta(\mathbf{r} - \mathbf{r}_i) \right\rangle = \int f_1(\mathbf{r}, \mathbf{v}, t) d\mathbf{v}, \quad (38)$$

to have a smaller value than specified, implying that the fluid phase may not have exactly the same properties as the pure solvent. In (38), $f_1(\mathbf{r}, \mathbf{v}, t)$ is the one-point distribution function.

In the present work, the number of solvent particles are kept unchanged when the colloidal particles are added. This measure is expected to lead to a fixed solvent number density (i.e., equal to 4 for any volume fraction of the colloidal phase). We will subject this to numerical tests through computing Eq. (38) over 400 bins that are non-overlapping and uniformly distributed in the 2D simulation box. Four sets of colloidal particles containing 9, 25, 49 and 81 suspended particles, which are, respectively, made up of 36, 100, 196 and 324 basic DPD particles (4 DPD particles per suspended particle), are added to the system. Figure 5 shows the distributions of the number density of the solvent across the channel. It can be seen that the solvent density is about 4 for all cases.

4.3 Spring force

Consider the case of a single colloidal particle. We observe that the spring forces on the constituent particles of the colloidal particle are oscillatory with zero mean and with a magnitude in the order of 10 (these forces are normalised with $a_{ij} = 18.75$, the maximum conservative force). However, the sum of these spring forces (i.e., the total force exerted on the colloidal particle) is very small in the order of 10^{-9} . One can anticipate such a result as the suspended particle base defined by the reference sites is assumed to have zero mass. These spring forces (of zero means) can be shown to have no contributions to the stress tensor.

4.4 Effective size of particles and volume fraction

We use the radial distribution function (RDF) [Reichl (1980)] to measure the exclusion or effective size of solvent and suspended particles

$$g(q) = \frac{1}{N/A} \frac{s}{2\pi q \Delta q} \text{ (for 2D)}, \quad g(q) = \frac{1}{N/V} \frac{s}{4\pi q^2 \Delta q} \text{ (for 3D)}, \quad (39)$$

where A/V is the area/volume (depending on the dimensionality of the problem) of the domain containing N particles and s is the number of particles in a circular/spherical shell of width $q \rightarrow (q + \Delta q)$ at a distance q from the centre of the particle under consideration. The total sum of the total exclusive volumes of all particles cannot be expected to be the same as the volume of the computational domain.

We investigate the effect of $k_B T$ (kinetic energy) on the particle size. Three values of $k_B T$, 0.25, 0.5 and 1, are considered. The variations of $g(q)$, where Δq is chosen as 0.01, for a solvent particle and a single suspended particle are shown in Figure 6 for 2D case and in Figure 7 for 3D case. Since q is the distance between the two particle centres, the effective radius can be estimated as $a_{eff}^S = \bar{q}/2$ for the solvent particle and $a_{eff}^C = \bar{q} - a_{eff}^S$ for the colloidal particle, where the superscripts S and C refer to solvent and colloidal particles, respectively, and \bar{q} is the value of q at which the RDF becomes non-zero - here since our resolution is chosen as $\Delta q = 0.01$, a non-zero RDF is deemed to occur at $g = 0.01$. Calculated values are listed in Table 1. It can be seen that the particle size increases as $k_B T$ is reduced. A larger particle size can be achieved at a negligible extra computational cost, contrasting with the frozen particle models, where one needs to employ a larger number of basic particles, and with the single particle models, where a larger cutoff radius may be required.

In the case of 3D particulate flows, the effective size of a solvent/colloidal particle can also be estimated via the Stokes-Einstein equation (done here as a consistency check only),

$$a_{eff} = \frac{k_B T}{6\pi\eta D}. \quad (40)$$

We estimate the self-diffusion coefficient

$$D = \frac{1}{6} \lim_{t \rightarrow \infty} \frac{d}{dt} \langle |\mathbf{r}_i(t) - \mathbf{r}_i(0)|^2 \rangle, \quad (41)$$

through the ensemble average of the mean square displacement (MSD) for a solvent particle and the time average of MSD for a single colloidal particle; the results are tabulated in Table 2. According to the kinetic theory approach, the effective size of a solvent particle is inversely proportional to $k_B T$ [Phan-Thien (2013)]. In numerical simulations, we also observe an increase in the particle size as $k_B T$ is reduced.

A comparison of the effective particle size, a_{eff} , from Tables 1 and 2 for the three values of $k_B T$, reveals that the RDF approach predicts larger values for a suspended particle and smaller values for a solvent particle than the Stokes-Einstein relation. It is noted that Brownian particles are usually of sizes typically several order of magnitudes greater than that of a solvent particle, so that solvent particles forces on a Brownian particle can be modelled by white noise impulses. It is expected that the Stokes-Einstein relation holds well for a large tagged particle moving in medium of much smaller particles. Our numerical results show that agreement between the Stokes-Einstein equation and the RDF approach is indeed consistently improved as the size of a tagged particle increases. At $k_B T = 0.25$, the effective size of a colloidal particle is 0.591 by the Stokes-Einstein equation and 0.675 by the RDF approach. We will use the RDF results, which are available for both circular discs (2D) and spheres (3D), in our calculations of particles sizes, providing the scaling factors in calculating Péclet number.

Table 1: No flow: effective sizes of solvent and colloidal particles measured by the radial distribution function.

$k_B T$	Solvent particle		Colloidal particle		
	\bar{q}	a_{eff}^S	\bar{q}	a_{eff}^C	a_{eff}^C/a_{eff}^S
Two dimensions					
1.0	0.01	0.005	0.4	0.3995	80
0.5	0.12	0.06	0.5	0.44	7.3
0.25	0.21	0.105	0.57	0.465	4.4
Three dimensions					
1.0	0.05	0.025	0.63	0.605	24
0.5	0.18	0.09	0.73	0.64	7.1
0.25	0.25	0.125	0.8	0.675	5.4

Table 2: No flow, 3D case: effective sizes of solvent and colloidal particles as predicted by the Stokes-Einstein relation.

$k_B T$	η	Solvent particle		Colloidal particle	
		D	a_{eff}	D	a_{eff}
Kinetic theory ($a_{ij} = 0$)					
1.0	2.4023	0.0870	0.2537	-	-
0.5	4.5000	0.0218	0.2709	-	-
0.25	8.9238	0.0054	0.2732	-	-
Numerical simulation ($a_{ij} = 18.75$, no flow)					
1.0	2.5106	0.12	0.1761	0.046	0.4594
0.5	4.5917	0.031	0.1864	0.011	0.5252
0.25	9.9830	0.0071	0.1871	0.00225	0.5905

As remarked earlier, DPD is a particle-based method, modelling a fluid behaviour so that in the end one satisfies conservation laws for the average quantities. A DPD particle is not supposedly a model of a discretised volume of the original liquid (in the sense of spatial techniques for solving continuum problems), and consequently we should not insist that the sum of exclusive volumes for the total DPD particles be equal to the original volume of liquid. This creates a problem for a definition of volume fraction in the case of a suspension. Since the aim is to solve a suspension problem for (21)-(22), we should insist that the definition of the volume fraction should lead to the celebrated Einstein's result (46) at low volume fractions. In our suspension model, with a total of N_C^0 basic DPD constituent particles used to represent the colloidal phase and N_S basic DPD particles used for the solvent phase, the particle fraction ($[PF]$) is defined as

$$[PF] = N_C^0 / (N_C^0 + N_S). \quad (42)$$

If a particle is associated with a volume (V_C^0 for a constituent particle and V_S for a solvent particle), then a candidate for the volume fraction may be

$$\phi = N_C^0 V_C^0 / (N_C^0 V_C^0 + N_S V_S). \quad (43)$$

In our case, $V_C^0 = V_S$, because of the standard DPD particles to represent both the constituent and solvent particles, then the volume fraction is the particle fraction.

We will demonstrate that (43) is a good candidate for a volume fraction definition for our case

where all the particles are of the same type. The test of this appropriate volume fraction definition is the satisfaction of the Einstein's relation (46) at low volume fraction, without any adjustment and irrespective of DPD parameters.

To connect this to the mass fraction, we may note that, if the constituent particle mass is m_C^0 , and the solvent particle mass is m_S , then in a uniform mixture of N_C^0 and N_S particles, the total mass of the system is

$$m_T = N_C^0 m_C^0 + N_S m_S. \quad (44)$$

This total mass makes up of a colloidal mass of $[MF]m_T = N_C^0 m_C^0$, and a solvent mass of $(1 - [MF])N_S m_S$, leading to the mass fraction $[MF]$,

$$[MF] = \frac{N_C^0 m_C^0}{N_C^0 m_C^0 + N_S m_S} = \frac{N_C^0 \rho_C}{N_C^0 \rho_C + N_S \rho_S}, \quad (45)$$

where ρ_S and ρ_C are the density of the solvent and the colloidal phases (this is because of $V_C^0 = V_S$). The mass fraction also reduces to volume fraction for the case where $\rho_S = \rho_C$.

4.5 Relative viscosity in Couette flow

For a dilute suspension of solid particles in d -dimensions, the reduced viscosity (the effective viscosity of the suspension divided by the viscosity of the suspending fluid) has been shown to be [Brady (1984)]

$$\eta_r = (1 + [\eta] \phi), \quad [\eta] = \frac{d+2}{2}, \quad (46)$$

where $[\eta]$ is the intrinsic viscosity, d the dimensions of hyperspheres in a viscous fluid and ϕ the volume fraction. $d = 3$ gives the celebrated Einstein's result $[\eta] = 2.5$ for 3D rigid spheres, and $d = 2$ gives $[\eta] = 2$ for 2D rigid cylinders.

We will now demonstrate that the use of (43) as a volume fraction is appropriate. Our numerical results at low volume fractions, for 2D cases, are displayed in Figure 8 for different colloidal mass and $k_B T$ values (the details of the simulation are reported below). It is seen that we obtain Einstein's results (46) at low volume fraction (less than 2.5%), pointed out the appropriate definition

of volume fraction (43). We note that only with the volume fraction defined as (43) do we recover Einstein’s results.

For concentrated suspensions, empirical and phenomenological studies have resulted in several relations for η_r as a function of ϕ . A well-known one is the equation proposed by Krieger and Dougherty (1959)

$$\eta_r = \left(1 - \frac{\phi}{\phi_m}\right)^{-\phi_m[\eta]} \quad (47)$$

where ϕ_m is the maximal packing fraction. This model is also expected to show a divergent behaviour (a rapid increase in the reduced viscosity) when ϕ_m is approached [Mewis and Wagner (2012)]. Quemada (1977) proposed the following equation deduced from the optimisation of viscous energy dissipation

$$\eta_r = \left(1 - \frac{\phi}{\phi_m}\right)^{-2}. \quad (48)$$

Relation (48) is a particular case of (47), where the exponent $-\phi_m[\eta]$ is set to 2. Note that the value of 2 was confirmed experimentally by van der Werff and de Kruif (1989). A theoretical construct by adding a dilute suspension of spheres of a certain size, then homogenize the suspension (resulting in a Newtonian fluid) before adding another dilute suspension of spheres of a greater size, etc., to build up a polydispersed suspension of spheres also yields (47) [Phan-Thien and Pham (1997)], with $\phi_m = 1$ and $[\eta] = 2.5$. This correlation (47) tacitly assumes that the suspension is Newtonian in its behaviour, so that its effective viscosity is independent of the shear rate, or that the correlated viscosity data are taken at a low shear rate, where there is not a significant amount of shear-rate dependence.

The maximal packing fraction ϕ_m is known to depend on the particle distribution, particle shape, etc., the more polydispersed the suspended phase, the higher is the maximal volume fraction; the effects of particles’ size on ϕ_m have been investigated by Metzner (1985) and Tsai et al. (1992). In the DPD method, monodisperse suspensions are modelled by using two groups of particles of two different sizes: one group of a smaller size representing the solvent phase and one group of a larger size representing the suspended phase. One can thus anticipate that the relative size ratio of suspended to solvent particles will have some influence on the maximal packing fraction in the DPD simulation. Figure 9 shows the smallest possible void created by three discs of a

radius a in contact in a highly packed structure. This triangular pore can be filled with a disc of a radius up to $a(2\sqrt{3} - 3)/3$. This leads to the condition that the smaller disc should be at least $3/(2\sqrt{3} - 3) \approx 6.46$ times smaller than the primary ones in order to avoid interfering in the original packing [Elliott et al. (2002)]. It is a necessary condition only - whether or not a maximal packing arrangement can be achieved would depend on the flow process as well. In the limit of a_{eff}^S/a_{eff}^C approaching zero, the maximal packing should be well-defined. The effects of the solvent particles sizes on the maximal packing fraction seem to be overlooked in previous DPD studies.

Our DPD results for the relative viscosity of the suspension are obtained through a simulation of Couette flow between two parallel plates. The Lees-Edwards [Lees and Edwards (1972)] periodic boundary condition is a mathematical device to implement a shear flow without having to do with solid boundaries. Its use leads to a suppression of density fluctuations near the wall, if solid walls are used and is adopted here. It is well known that monodisperse hard spheres undergo an equilibrium phase transition at $\phi \approx 0.494$ to a crystalline structure [Foss and Brady (2000)]. At large concentration, $\phi > 0.5$, the velocity profile can be nonlinear with respect to the shear coordinate. In this work, the volume fraction is considered in a range of 0 to 0.49 for 3D flows and 0 to 0.55 for 2D flows. The viscosity is simply computed as $\eta = S_{xz}/\dot{\gamma}$, where S_{xz} is the shear component of the stress tensor and $\dot{\gamma}$ the imposed shear rate. To compare with published data on the reduced viscosity, we use the lowest shear rate that still yields stable results (0.01 for 2D and 0.0075 for 3D) for which shear-rate dependence will not be a concern - shear thinning behaviour will be explored later.

2D case: For equal discs in the plane, the hexagonal packing is known to yield the highest packing fraction $\pi/\sqrt{12} \approx 0.91$ [Mewis and Wagner (2012)]. Figure 10 shows our reduced viscosity results at $k_B T = 1$. Krieger-Dougherty and Quemada equations, where $\phi_m = 0.91$ is used, and other results using the fictitious-domain/finite-element method [Hwang et al. (2004)] and the smoothed particle hydrodynamics (SPH) method [Bian and Ellero (2014)] for the range of ϕ under consideration are also included for comparison. It is noted that short-range lubrication forces are included explicitly in the SPH simulation. The present results are in good agreement with those predicted by Krieger-Dougherty model using $\phi_m = 0.91$. When the maximal packing fraction is chosen lower (e.g., $\phi_m = 0.87$), the relative viscosity predicted by empirical models become

divergent at a relatively lower ϕ value (as compared to that when $\phi_m = 0.91$). Such a behaviour is also observed in the present simulation when $k_B T$ is reduced from 1 to 0.5. Reducing $k_B T$ also increases solvent particles' size (Table 1). The ratio of the effective size of the colloidal particle to that of the solvent particle reduces from 80 for $k_B T = 1$ to 7.3 for $k_B T = 0.5$. Such a quick decrease in the radius ratio is expected to reduce the maximal packing fraction. Our results at $k_B T = 0.5$ are close to those predicted by SPH [Bian and Ellero (2014)].

3D case: For a suspension of monosized spherical particles, the maximal packing fraction is found to be 0.71 for hexagonal packing and 0.65 for random close packing, which are significantly lower than the values for 2D case. As shown in Figure 11, our results with $k_B T = 1$ agree well with Krieger-Dougherty model using $\phi_m = 0.65$ and also with the experimental data by van der Werff and de Kruif (1989). Decreasing $k_B T$ results in a faster increase in the ratio of solvent particles to colloidal particles sizes (Table 1). The ratio a_{eff}^C/a_{eff}^S is reduced from 24.2 for $k_B T = 1$ to 7.1 for $k_B T = 0.5$. As a result, the maximal packing fraction is expected to decrease as $k_B T$ is reduced. Our relative viscosity for $k_B T = 0.5$ is found to fit better empirical models with a lower effective maximal packing fraction (than $\phi_m = 0.65$).

In the work of Pan et al. (2010a), the effective radii of the colloidal and solvent particles were reported to be 0.98 and 0.27, respectively. The ratio of the former to the latter is thus 3.6 only, which appears not to be large enough for an effective maximal packing fraction of 0.65 to take place. However, their results concerning the relative viscosity are in good agreement with the empirical predictions employed with $\phi_m = 0.65$.

Since the relative size ratio between solvent to suspended particles can affect the maximal packing, it can be controlled in particle-based methods. In our model, the suspended particle size can be adjusted by means of its constituent particles. Larger sizes are achieved by simply increasing the number of constituent particles. Through numerical experiments, we have observed that (i) the size of solvent particles is significantly reduced as $k_B T$ increases (e.g., 21 times when one increases $k_B T$ just 4 times (Table 1)); and (ii) the size of solvent particles is quite small at large values of $k_B T$ (e.g., 0.005 at $k_B T = 1$ (Table 1)). Also note that the effects of compressibility will be reduced as $k_B T$ increases [Pan et al. (2013)]. The ratio of the effective size of the colloidal particle

to that of the solvent particle can be made large with increasing $k_B T$ and/or increasing the size of colloids. The preferred alternative is to use more constituent particles per suspended particle to represent a larger suspended particle. As an example, if the colloid is designed with $a_{eff} \approx 0.5$ and solvents with $a_{eff} = 0.005$ (Table 1 ($k_B T = 1$)), this ratio will be about 100 - this ratio is sufficient to maintain the maximal packing fraction that is customarily reported; a further increasing $k_B T$ beyond this will not affect the maximal packing fraction.

4.6 Shear thinning behaviour

We consider the shear rate in the range of [0.05-10] for $k_B T = 1$ and [0.01-10] for $k_B T = 0.5$ in 2D, and [0.01-10] for $k_B T = 1$ and [0.0075-10] for $k_B T = 0.5$ in 3D. For shear flows, compressibility effect is not a significant factor and therefore Mach number may not be relevant. However, we can define Mach number as $Ma = v/c$, where $v = \dot{\gamma} a_{eff}^C$ is a typical velocity, and c is the sonic velocity. The corresponding Mach number is in the range of [0.004-0.87] for $k_B T = 1$ and [0.001-0.98] for $k_B T = 0.5$ in 2D, and [0.001-1.35] for $k_B T = 1$ and [0.001-1.58] for $k_B T = 0.5$ in 3D. The corresponding Reynolds number, defined as $\rho_s v L / \eta_s$, where L is the channel width, is in the range of [0.005-1.02] for $k_B T = 1$ and [0.001-0.65] for $k_B T = 0.5$ in 2D, and [0.002-2.91] for $k_B T = 1$ and [0.001-1.78] for $k_B T = 0.5$ in 3D. The suspension viscosity as a function of the Péclet number for two values of $k_B T$ are plotted in Figure 12 for 2D and in Figure 13 for 3D. Each data point in these plots is the average value of results acquired from ten independent runs/simulations - each run is comprised of 200,000 time steps for 2D and 300,000 time steps for 3D. For both 2D and 3D cases, a shear-thinning behaviour is observed and its strength increases as $k_B T$ is reduced. For a given time step, a specified temperature is better maintained at low Pe , while the solution converges faster at high Pe . Deviation (from the run statistics) is found to be small at high Pe and large at low Pe . DPD results for lower shear rates than the lowest recorded here, are found not to improve much by taking longer runs.

4.7 Normal stress differences

First and second normal stress differences are defined as $N_1 = S_{xx} - S_{zz}$ and $N_2 = S_{zz} - S_{yy}$, respectively. For 2D, one is able to compute N_1 only. Non-zero normal stress differences are a manifestation of non-Newtonian characters of the fluid. The Couette flow is simulated with the Lees-Edwards periodic boundary conditions, in which normal stress differences are computed by two different formulas for a consistency check, namely the Irving-Kirkwood (IK) formula and the formula that uses the normal forces for the case of two parallel plates in shear. The IK formula involves not only forces but also velocities throughout the computational domain, while the wall force-like approach needs only values of the pairwise forces across the top plane.

Irving-Kirkwood's expression: We use (16) to compute the normal stress differences and display the 3D results for $k_B T = 1$ and 0.5 in Figures 14-15, respectively. It can be seen that the present variations of N_1 and N_2 with respect to Pe are similar in behaviour to those obtained by the Stokesian Dynamics [Foss and Brady (2000)]. There are two contributions to the stress tensor, namely Brownian and hydrodynamic. As discussed in [Foss and Brady (2000)], the hydrodynamic contributions are negative for all values of Pe while the Brownian contribution is positive for N_1 and negative for N_2 . It is noted that when Pe approaches zero, due to flow-reversal symmetry requirement, both N_1 and N_2 vanish. At low Pe numbers, the Brownian contribution is strong and dominates the behaviour. In Figures 14-15, at low Pe , the first normal stress difference is observed to be positive and the second normal stress difference negative as expected. Results also indicate that both normal stress differences are of comparable magnitude. As Pe increases, the effects of hydrodynamic forces become an important factor, and N_1 is observed to change from positive to negative at $Pe = O(10)$. After this point, hydrodynamics dominate and both normal stress differences are both to be negative. Although the trend in all the simulations, ours, Foss and Brady (2000), and Pan et al. (2010a) are similar, a quantitative agreement is lacking, pointing out the need for more studies in this particular area.

Wall force-like approach: The non-Newtonian character of the suspension is evidenced by the presence of normal forces on the walls. One can calculate N_1 and S_{xz} in the form: $N_1 = -F_z^w/A^w$ and $S_{xz} = F_x^w/A^w$, where F_z^w and F_x^w are the z and x components of the total force vector on

the wall (the plane normal to the z axis) and A^w the area of the wall under consideration in the simulation. The boundary traction is calculated through $\mathbf{t} = \mathbf{S}\mathbf{n}$ with \mathbf{n} being the outward unit normal vector of the boundary. It thus leads to $F_z^w = \int_{A^w} S_{zz}^w dA^w = (-\bar{p} + \bar{T}_{zz}^w)A^w$, where \bar{p} is the isotropic part of the stress tensor and the bar over symbols denotes a mean value. Since there are no external forces on the fluid in the flow direction, one has, on the downstream plane, $F_x^d = \int_{A^d} S_{xx}^d dA^d = (-\bar{p} + \bar{T}_{xx}^d)A^d = 0$ or $-\bar{p} = -\bar{T}_{xx}^d$, where the superscript d is used to denote the downstream surface (the plane normal to the x axis). Expression for the normal force on the wall can be rewritten as $F_z^w = (\bar{T}_{zz}^w - \bar{T}_{xx}^d)A^w$. If stresses are assumed to have a uniform distribution on a boundary, one has $F_z^w/A^w = S_{zz} - S_{xx} = -N_1$. Figure 16 compares N_1 and σ_{xz} in 3D between the Irving-Kirkwood expression and the wall force-like approach. With a good agreement achieved, we conclude that our normal stress data are internally consistent.

4.8 Migration of colloidal particles in Poiseuille flow

The cross-streamline shear-induced migration of suspended particles has attracted a great deal of attention because of its practical importance in various industrial applications such as paper coating and food processing [Phillips et al. (1992); Phan-Thien et al. (1995)]. Here, we just want to report a quick application of the model in this area without an exhaustive review. In general, for an inhomogeneous shear flow of a suspension, it has been observed that suspended particles migrate towards a region of a lower shear rate. There have been several theories of this migration phenomenon, but we want to focus on Phillips et al.'s (1992) theory, in which a constitutive model for the shear-induced migration of particles consisting of a flux of particles away from the collision events and a flux away from the concentration gradient was proposed. The balance of these produces a concentration profile satisfying

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \nabla \cdot \mathbf{N}, \quad (49)$$

where \mathbf{N} is the flux of particles

$$\mathbf{N} = K_c a^2 \phi \nabla (\dot{\gamma} \phi) + K_\eta a^2 \dot{\gamma} \phi^2 \nabla (\ln \eta), \quad (50)$$

in which K_c and K_η are phenomenological constants, $\dot{\gamma}$ is the generalised strain rate, a is a particle size, and η is the suspension viscosity. Together with the assumption of a Newtonian suspension, and a Krieger-Dougherty model for its viscosity, this constitutive theory has been tested out in some flow configuration (e.g., [Phan-Thien et al. (1995)]).

In a plane Poiseuille flow, eq. (49) yields an implicit relation for the concentration:

$$\frac{\phi}{\phi_w} \left(\frac{\eta_w}{\eta} \right)^{1-K_\eta/K_c} = \frac{h}{\xi}, \quad (51)$$

where ξ is the coordinate axis ($\xi = 0$ is the centreline, and $\xi = h$ is the wall), and the subscript w defines a wall quantity.

To obtain a solution from (49), a specific constitutive form for the stress must be adopted in the balance of momentum equation in order to calculate the velocity field.

We are interested in finding out if our DPD model can yield some shear-induced migration data, and thus the pressure driven flow between two parallel infinite planes is chosen as a test problem. Particles are expected to move from the walls (high shear) to the centre of the channel (low shear), according to Phillips et al.'s (1992) theory. This flow can be effectively simulated in a reverse Poiseuille flow configuration, by imposing periodic conditions on all boundaries [Backer et al. (2005)]. Initially, a uniform arrangement of particles is formed. Their motion is then driven by applying a body force $\mathbf{F} = (g, 0, 0)^T$ to each particle in the upper region (i.e., $z > 0$) and $\mathbf{F} = (-g, 0, 0)^T$ to each particle in the lower region (i.e., $z < 0$). This automatically generates a counter-flowing Poiseuille flow through periodic boundary conditions, without the use of frozen wall particles at the boundaries. The simulation is carried out with $g = 0.4$ and 1.0 . After 300,000 time steps, we compute local concentrations and plot them as functions of distance across the channel in Figure 17. It can be seen that local concentrations are higher at the centre of the channel as the flow rate is increased (the maximum velocity is 3.94 for $g = 0.4$, and 11.32 for $g = 1$).

Eq. (51) for a suspension at volume fraction of 43% can be tested using the DPD data for ϕ_w and the simulated local suspension viscosity, and $K_\eta/K_c = 3.77$. (51) then represents an implicit non-linear

equation in ϕ , which can be solved using a library routine in MATLAB; the results are included in Figure 17 (as solid lines labelled "Analytic model"); in both cases, the average concentration, determined by a post-integration of the volume fraction, is $\bar{\phi} = 0.43$. The agreement in the volume fraction profiles, from the DPD data and Phillips et al.'s (1992) results, cannot be maintained for the same ϕ_w and K_η/K_c , for both cases studied here. In order to have good agreement in both cases, we must allow either ϕ_w or K_η/K_c to be changed. We opt to change ϕ_w , from 0.28 (DPD's data) to 0.32 in the case where $g = 1$, and the agreement is good for both sets of results. Our data appear to support several main features of the Phillips et al.'s model including the concentration approaching ϕ_m at the centreline. Note that Phillips et al.'s (1992) theory has been tested without the need to specify any particular constitutive equation here. The agreement, even without adjusting ϕ_w , is reasonable, suggesting that the simple migration model (49) is useful and captures the main features of interest.

The cross-streamline migration of suspended particles is expected to lead to a change in the flow behaviour. As shown in Figure 18, the present velocity profile is no longer parabolic. It flattens in the region near the centre and steepens in the region near the wall. Our results are comparable to those of previous studies (e.g., [Pan et al. (2010a)]).

4.9 Time step and temperature

All simulations presented in this study are conducted with $\Delta t = 0.01$ for 2D and $\Delta t = 0.001 - 0.005$ for 3D. It was reported in [Pan et al. (2010a)], where an exponential form for the conservative force is employed, the time step used for their simulation of colloidal suspensions in 3D was in the range of 0.0002 to 0.0005 in order to maintain the temperature at $k_B T = 1.0$. The present model thus allows one to use a relatively large time step.

Figure 19 compares the obtained average thermodynamic temperature for various values of the volume fraction between the frozen particle model and the present model. It can be seen that the former is not able to maintain well the desired temperature over the flow domain as the volume fraction increases. In contrast, the percentage error of our model is less than 8% for all values of

the volume fraction employed.

5 Concluding Remarks

DPD is a particle-based simulation method that satisfies conservation of mass and momentum. Like other simulation methods (e.g., finite volume methods (FVMs) and finite element methods (FEMs)), the DPD method produces field results that satisfy the Navier-Stokes equations, and can be regarded in some physical sense as a particle-based discretisation of the Navier-Stokes equations. The position and velocity of DPD particles can be solved individually (without the need to construct the global system matrix as done in FVMs and FEMs). The drawbacks are the issues of resolution, requiring the use of very large numbers of particles to represent the flow, and of ignoring phenomena below the length scale of a particle. The most powerful strength of DPD lies in its ability to model complex-structured fluids in a simple way. DPD particles can be connected to form chains to model polymer solutions, to form rigid particles to model suspensions, to form immiscible droplets to model multiphase fluids, to form membranes encapsulating another fluid to model biological cells, etc. In the present study, we propose a simple but effective way to construct suspended rigid particles. In the proposed model, we replace the solvent by DPD particles using the standard DPD parameters ($n = 4$, $a_{ij} = 18.75$, $\sigma = 3$, $r_c = 1$ and $k_B T = 1$), and link up a small number of some DPD particles by springs to form suspended particles. The spring stiffness is chosen large (e.g., 3000 in this study) to ensure a good representation of rigid particles. We have found that decreasing $k_B T$ (a measurement of kinetic energy) from unity, while keeping the other DPD parameters constant, affects the particles exclusion sizes, which produces a significant change in the suspended to solvent particles size ratio, and thus directly affects the maximal packing fraction. The size effect of the solvent particles seems to have been overlooked in previous DPD publications. Special care is thus needed in ensuring that the suspended to solvent size ratio is sufficiently large in order to have a similar to observed maximal packing fraction (ϕ_{max}). In the proposed model, we have presented in detail the calculation of volume fraction and number density, and also demonstrated its improvement, particularly in time step and simplicity over the single particle model, and in the system size and temperature variation over the frozen

particle model. In particular, we have demonstrated that

- the solvent number density remains constant and thus insures that the solvent properties remain unchanged for any volume fraction of the suspension phase;
- the spring forces do not make any contributions to the stress tensor;
- a specified Boltzmann temperature can be maintained throughout the entire domain with the help of the spring forces, and this parameter is found to account for the strength of shear-thinning behaviour of the suspension and for the effective maximal packing fraction;
- the suspended/solvent size ratio increases with the temperature.

In spite of its simplicity, the present model is able to yield a good prediction of the zero-shear-rate relative viscosity over a wide range of the volume fraction. The trend in the normal stress differences versus shear rate is similar to other previous studies, but we do not have a quantitative agreement across all the methods (Stokesian Dynamics Simulation and other DPD methods). This will need further studies. The present model also produces the expected cross-streamline particle migration from high shear to low shear regions, in agreement with Phillips et al. (1992) shear-induced migration theory; more detailed studies on the shear-induced migration phenomena with DPD method should be a welcome contribution, in particular in the area of highly dispersed and non-Newtonian suspensions, where DPD has its distinct advantages of being able to model suspended particles of different sizes and viscoelastic solvents with relative ease.

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References

1. Backer, J. A., C. P. Lowe, H. C. J. Hoefsloot, and P. D. Iedema, "Poiseuille flow to measure the viscosity of particle model fluids," *Journal of Chemical Physics* **122**, 154503 (2005).
2. Bian, X., and M. Ellero, "A splitting integration scheme for the SPH simulation of concentrated particle suspensions," *Computer Physics Communications* **85**(1), 53-62 (2014).
3. Bian, X., S. Litvinov, R. Qian, M. Ellero, and N. A. Adams, "Multiscale modeling of particle in suspension with smoothed dissipative particle dynamics," *Physics of Fluids* **24**, 012002 (2012).
4. Bicerano, J., J. F. Douglas, and D. A. Brune, "Model for the Viscosity of Particle Dispersions," *Journal of Macromolecular Science, Part C: Polymer Reviews* **39**(4), 561-642 (1999).
5. Boek, E. S., P. V. Coveney, H. N. N. Lekkerkerker, and P. van der Schoot, "Simulating the rheology of dense colloidal suspensions using dissipative particle dynamics," *Phys. Rev. E* **55**(3), 3124-3133 (1997).
6. Brady, J. F., "The Einstein viscosity correction in n dimensions," *International Journal of Multiphase Flow* **10**(1), 113-114 (1984).
7. Chen, S., N. Phan-Thien, B. C. Khoo, and X.-J. Fan, "Flow around spheres by dissipative particle dynamics," *Phys. Fluids* **18**(10), 103605 (2006).
8. Clark, A. T., M. Lal, J. N. Ruddock, and P. B. Warren, "Mesoscopic simulation of drops in gravitational and shear fields," *Langmuir* **16**(15), 6342-6350 (2000).
9. Dzwinel, W., and D. A. Yuen, "A two-level, discrete-particle approach for simulating ordered colloidal structures," *Journal of Colloid and Interface Science* **225**1, 179-190 (2000).
10. Einstein, A., "Eine neue Bestimmung der Moleküldimensionen", *Ann. Phys.* **19**, 298-306 (1906). Reprinted in "Investigations on the theory of the Brownian movement," Edited by R. Furth, Translated by A.D. Cowper, Dover, New York (1956).
11. Elliott, J. A., A. Kelly, and A. H. Windle, "Recursive packing of dense particle mixtures," *Journal of Materials Science Letters* **21**(16), 1249-1251 (2002).

12. Español, P., “Hydrodynamics from dissipative particle dynamics,” *Phys. Rev. E* **52**, 1734-1742 (1995).
13. Español, P., and M. Revenga, “Smoothed dissipative particle dynamics,” *Phys. Rev. E* **67**(2), 026705 (2003).
14. Español, P., and P. Warren, “Statistical mechanics of dissipative particle dynamics,” *Europhysics Letters* **30**(4), 191-196 (1995).
15. Fan, X., N. Phan-Thien, S. Chen, X. Wu, and T. Y. Ng, “Simulating flow of DNA suspension using dissipative particle dynamics,” *Phys. Fluids* **18**(6), 063102 (2006).
16. Foss, D. R., and J. F. Brady, “Structure, diffusion and rheology of Brownian suspensions by Stokesian Dynamics simulation,” *J. Fluid Mechanics* **407**, 167 (2000).
17. Gatsonis, N. A., R. Potami, and J. Yang, “A smooth dissipative particle dynamics method for domains with arbitrary-geometry solid boundaries,” *Journal of Computational Physics* **256**, 441-464 (2014).
18. Groot, R. D., “How to impose stick boundary conditions in coarse-grained hydrodynamics of Brownian colloids and semi-flexible fiber rheology,” *J. Chem. Phys.* **136**, 064901 (2012).
19. Groot, R. D., and P. B. Warren, “Dissipative particle dynamics: Bridging the gap between atomistic and mesoscopic simulation,” *J. Chem. Phys.* **107**, 4423 (1997).
20. Hoogerbrugge, P. J., and J. M. V. A. Koelman, “Simulating microscopic hydrodynamic phenomena with dissipative particle dynamics,” *Europhysics Letters* **19**(3), 155-160 (1992).
21. Hwang, W. R., M. A. Hulsen, and H. E. H. Meijer, “Direct simulation of particle suspensions in sliding bi-periodic frames,” *J. Computational Physics* **194**, 742-772 (2004).
22. Irving, J. H., and J. G. Kirkwood, “The statistical mechanical theory of transport processes. IV. The equations of hydrodynamics,” *J. Chem. Phys.* **18**, 817 (1950).
23. Jamali, S., M. Yamanoi and J. Maia, “Bridging the gap between microstructure and macroscopic behavior of monodisperse and bimodal colloidal suspensions,” *Soft Matter* **9**, 1506-1515 (2013).

24. Jiang, W., J. Huang, W. Yongmei, and M. Laradji, "Hydrodynamic interaction in polymer solutions simulated with dissipative particle dynamics," *J. Chem. Phys.* **126**, 044901 (2007).
25. Koelman, J. M. V. A., and P. J. Hoogerbrugge, "Dynamic simulations of hard-sphere suspensions under steady shear," *Europhysics Letters* **21**(3), 363-368 (1993).
26. Kong, Y., C. W. Manke, W. G. Madden, and A. G. Schlijper, "Effect of solvent quality on the conformation and relaxation of polymers via dissipative particle dynamics," *J. Chem. Phys.* **107**, 592 (1997).
27. Krieger, I. M., and T. J. Dougherty, "A mechanism for non-Newtonian flow in suspensions of rigid spheres," *Trans. Soc. Rheol.* **3**, 137 (1959).
28. Kulkarni, P. M. and C.-C. Fu, M. S. Shell, and L. Gary Leal, "Multiscale modeling with smoothed dissipative particle dynamics," *The Journal of Chemical Physics* **138**, 234105 (2013).
29. Laradji, M., and M. J. A. Hore, "Nanospheres in phase-separating multicomponent fluids: A three-dimensional dissipative particle dynamics simulation," *J. Chem. Phys.* **121**, 10641 (2004).
30. Lees, A. W., and S. F. Edwards, "The computer study of transport process under extreme conditions," *J. Phys. C* **5**, 1921 (1972).
31. Mai-Duy N., D. Pan, N. Phan-Thien, and B. C. Khoo, "Dissipative particle dynamics modelling of low Reynolds number incompressible flows," *J. Rheol.* **57**(2), 585 (2013).
32. Marsh, C. A., *Theoretical Aspects of Dissipative Particle Dynamics*, (PhD thesis), (University of Oxford, Oxford, 1998).
33. Marsh, C. A., G. Backx, and M. H. Ernst, "Static and dynamic properties of dissipative particle dynamics," *Phys. Rev. E* **56**(2), 1676-1691 (1997).
34. Martys, N. S., "Study of a dissipative particle dynamics based approach for modeling suspensions," *J. Rheol.* **49**, 401 (2005).
35. Metzner, A. B., "Rheology of suspensions in polymeric liquids," *J. Rheol.* **29**, 739 (1985).

36. Mewis, J., and N. J. Wagner, *Colloidal Suspension Rheology*, (Cambridge University Press, London, 2012).
37. Nikunen, P., I. Vattulainen, and M. Karttunen, “Reptational dynamics in dissipative particle dynamics simulations of polymer melts,” *Phys. Rev. E* **75**(3), 036713 (2007).
38. Novik, L., and P. Coveney, “Using dissipative particle dynamics to model binary immiscible fluids,” *Int. J. Mod. Phys. C* **8**(4), 909-918 (1997).
39. Pan, W., B. Caswell, and G. E. Karniadakis, “Rheology, microstructure and migration in Brownian colloidal suspensions,” *Langmuir* **26**(1), 133-142 (2010a).
40. Pan, W., B. Caswell, and G. E. Karniadakis, “A low-dimensional model for the red blood cell,” *Soft Matter* **6**, 4366-4376 (2010b).
41. Pan, D., N. Phan-Thien, N. Mai-Duy, and B. C. Khoo, “Numerical investigations on the compressibility of a DPD fluid,” *Journal of Computational Physics* **242**, 196-210 (2013).
42. Pan, W., I. V. Pivkin, and G. E. Karniadakis, “Single-particle hydrodynamics in DPD: A new formulation,” *EPL* **84**(1), 10012 (2008).
43. Phan-Thien, N., *Understanding Viscoelasticity - An Introduction to Rheology*, (Second Edition), (Springer, Berlin, 2013).
44. Phan-Thien, N., A. L. Graham, S. A. Altobelli, J. R. Abbott, and L. A. Mondy, “Hydrodynamic particle migration in a concentrated suspension undergoing flow between rotating eccentric cylinders,” *Ind. Eng. Chem. Res.* **34**, 3187-3194 (1995).
45. Phan-Thien, N., and D. C. Pham, “A differential multiphase models for polydispersed suspensions and particulate solids,” *J. non-Newt. Fluid Mech.* **72**, 305-318 (1997).
46. Phillips, R. J., R. C. Armstrong, R. A. Brown, A. L. Graham, J. R. Abbott, “A constitutive equation for concentrated suspensions that account for shear-induced particle migration,” *Phys. Fluids* **4**, 30-40 (1992).
47. Pryamitsyn, V., and V. Ganesan, “A coarse-grained explicit solvent simulation of rheology of colloidal suspensions,” *J. Chem. Phys.* **122**, 104906 (2005).

48. Quemada, D., "Rheology of concentrated disperse systems and minimum energy dissipation principle," *Rheologica Acta* **16**(1) 82-94 (1977).
49. Reichl, L. E., *A Modern Course in Statistical Physics*, (University of Texas Press, Austin, Texas, 1980).
50. Sierou, A., and J. F. Brady, "Accelerated Stokesian Dynamics simulations," *J. Fluid Mechanics* **448**, 115-146 (2001).
51. Tsai, S. C., D. Botts, and J. Plouff, "Effects of particle properties on the rheology of concentrated noncolloidal suspensions," *J. Rheol.* **36**, 1291 (1992).
52. van der Werff, J. C., and C. G. de Kruif, "Hard-sphere colloidal dispersions: the scaling of rheological properties with particle size, volume fraction, and shear rate," *J. Rheol.* **33**, 421 (1989).
53. Whittle, M., and K. P. Travis, "Dynamic simulations of colloids by core-modified dissipative particle dynamics," *J. Chem. Phys.* **132**, 124906 (2010).
54. Ye, T., Phan-Thien, N., Khoo, B.C., and Lim, C.T., "Stretching and relaxation of malaria-infected red blood cells," *Biophysical J*, **105**, 1103-1109 (2013).

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