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Predicting rheology of suspensions of spherical and non-spherical particles using dissipative particle dynamics (DPD): methodology and experimental validation

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The rheology of non-dilute colloidal suspensions is a complex phenomenon and predictive numerical methodologies for it are still in the emerging phases. Dissipative particle dynamics (DPD), a particle-based numerical scheme for phenomena in the mesoscopic regime, has emerged as an attractive technique to tackle this problem. In this article, a practical methodology for using DPD for quantitative prediction of the rheology of non-dilute suspensions is presented and validated with focused, specific experiments. Some pertinent issues are highlighted to make DPD more amenable to being a computational tool for practical applications. The presence of solid particles of disparate sizes and non-spherical geometries poses special challenges. Methodologies to address them are presented with validations and efficient techniques are suggested to make them computationally amenable.

Keywords: dissipative particle dynamics; bounce-back condition; rheology

1. Introduction

The rheology of non-dilute suspensions is an extremely complex phenomenon to predict, primarily due to the following two factors [1,2,3]: (a) the vast range of length scales (few nanometers to hundreds of microns) involved, and (b) the presence of hydrodynamic forces as a critical factor. Many dedicated numerical techniques have emerged to address this problem over the past few decades with limited success. Particle-based techniques like Brownian and Stokesian dynamics [1,4] are severely limited in their ability to handle high solid concentrations and high shear rates. This is due to inherent limitations such as the lack of satisfaction of Galilean invariance and also non-scalability of computations for large systems [1]. Lattice-based techniques such as the Lattice–Boltzman technique have severe limitations too, primarily stemming from the presence of the lattice and the lack of unconditional satisfaction of Galilean invariance [1]. In the past few years dissipative particle dynamics (DPD) has emerged as an attractive numerical technique for predicting the rheology of these systems [5]. The attractiveness of DPD comes from its pure-particle nature and its natural ability to handle the hydrodynamic effects that can dominate these systems [1,5].

The fundamental aspects of DPD and how it can be applied to dilute suspensions are presented in references [1,2,5]. In this paper, the DPD formulation is further expanded for non-dilute suspensions and validated using experiments. Relevant discussions on spatial and temporal scale considerations are presented in the

process to make the use of DPD for real-life applications more intimate and predictive. In this spirit, mitigating the computational intensiveness of DPD is kept in mind in order to facilitate its use for practical problems.

The presence of solid particles with complex (non-spherical) geometries makes computational modelling more difficult and cumbersome. Owing to the preponderance of hydrodynamic effects in these systems, particle shape and size have a considerable effect on macroscopic rheology. Therefore, accounting for them within the framework of DPD is a challenge. A freezing technique in which a large solid particle is constructed out of smaller spherical particles by aggregating them as a rigid entity is commonly employed for modelling non-spherical particles of disparate sizes [2,5]. In this article, this technique is further refined. It is seen that an improper implementation of this freezing technique can give rise to local, spurious effects, which, if not addressed, can lead to errors in viscosity calculations.

In the remainder of this paper the experiments are first described followed by the description of the ‘non-freezing’ DPD formulation and its comparison with experiments. The freezing technique is then taken up for some elaboration followed by conclusions.

2. Experiments

The experiments were performed with a cone-plate viscometer that can maintain a constant shear rate. A simple schematic of the viscometer is shown in Figure 1.

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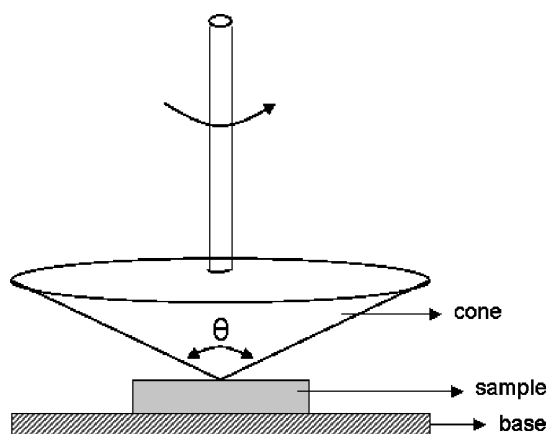


Figure 1. A simple schematic of a cone-plate viscometer.

The sample is placed between the cone and the rigid planar base. The cone is rotated at programmed speeds (that maintains the shear rate) and the measured torque is the measure of the viscosity of the sample. When the cone angle ' θ ' is 180 then it becomes a parallel plate viscometer.

Two different samples of water-based suspension from Bang Laboratories were used. They were: (1) 10% (by weight) of mono-disperse, spherical Poly-Styrene (PS) beads of $0.95\ \mu\text{m}$ diameter, and (2) 30%, mono-disperse PS beads of the same size. PS has a density that is close to water and care was taken to make the suspensions well dispersed when the experiments were performed. The dynamic rheometer, MCR-300 from Anton-Paar Physica, fitted with the largest plates available (50 mm in diameter) with an average 1 mm gap, was used in order to maximise the torque outputs [6]. The shear rate was varied from 10/s to 7500/s, with a total of 12 steps spaced logarithmically. To minimise water evaporation during the test and to maximise the data acquisition time for each shear rate, a compromise was made at 30 s per data point for the lowest shear rate, and 3 s at the highest shear rate. The total test time was therefore programmed to be under 200 s. The viscometer was first calibrated by measuring the known viscosity of water ($\sim 1\ \text{cP}$) at 23.0°C , the temperature at which all suspension measurements were also made.

3. Comparison with mono-disperse cases

Within the DPD framework the solid particles can be treated either as frozen aggregates of unit DPD particles or, if possible, as individual computational entities [13,14]. The former technique is more prevalent and versatile but has the disadvantage of increasing the total number of particles, as will be discussed in detail later in this article. The latter technique is not viable for complex

particle shapes and particles of large sizes. This is due to the fact that a unitary, centre-to-centre, pair-wise interaction does not adequately represent size and shape factors which are important in rheology due to the hydrodynamic effects [4]. However, our work has shown that for suspensions with spherical solid particles up to a micron in diameter, the particles could be treated as unit computational entities without sacrificing accuracy if the interaction between the solid particles is chosen correctly. Since the mono-disperse experimental samples used here had particles of sub-micron size ($0.95\ \mu\text{m}$), it was decided that they should be treated as a single solid body. Later in this article a comparison with the freezing approach will be presented as further validation. Consequently, there are two distinct types of computational particles in this DPD formulation – fluid particles representing the fluid (or the solvent), and the solid particles (larger in size than the fluid particles) representing the solute.

Because of the nature of the materials in the system and non-dense solid loading fractions a hard sphere suspension model [8] was used wherein hydrodynamic interactions are predominant over non-hydrodynamic interactions like electrostatics. The interaction between the solid particles was further augmented by the repulsive 'Electric Double-layer' (EDL) force in the DLVO family of the form given in Equation (1) below, that takes into consideration the material properties of the solvent (water) and the solid (PS in this case) [7]. At these levels of solid packings, and given the passive nature of the solvent, – in the spirit of a hard-sphere model – it is believed that hydrodynamic interactions outweigh other non-hydrodynamic effects.

$$F(r) = F_0 \exp(-\kappa h) \quad h < r_c. \quad (1)$$

In Equation (1) r_c is the cut-off radius, h is the distance between the surfaces of the solids and F_0 and κ are material specific properties [7]. Inverse of κ is the Debye length, which primarily depends on the ionic strength of the solvent. F_0 encompasses properties like κ , solid surface potential, relative permittivity of solvent, etc. For details on these parameters readers are referred to Israelachvili [7]. In accordance with the experiments the properties used in this work pertain to a suspension of polystyrene in water with an ionic strength of $10^{-2}\ \text{M}$. κ also signifies the range parameter of the colloidal interaction, which is typically of a smaller range than r_c . It should be noted, therefore, that specific material properties are being employed in this DPD formulation in an attempt to render this technique a predictive, quantitative tool for practical use.

Standard DPD forces and parameters were used for the interaction between the fluid particles [2,12]. Between the fluid and solid particles, for the

conservative force [see Equation (4) below], a value of a_{ij} of around $a_{ff}/2$ was found to be appropriate, with a_{ff} being the fluid–fluid counterpart. Since this is a hard-sphere model these conservative terms have a secondary effect on reduced viscosities. The role of the coefficient of dissipative force term between solid and fluid particles was found to be limited. Long-term simulations showed that it had no practical effect on reduced viscosity so the standard value of 5.6 was used [12]. Finally, for the interaction between the solid particles, since the particles are rigid, the dissipation force term was set to zero and for the conservative repulsion force Equation (1) was used as explained earlier. All the different types of forces between the constituents are summarised in Table 1.

3.1 Computational considerations

A standard DPD non-dimensionalization scheme was used [2] where distances are non-dimensionalised with respect to the cut-off radius (r_c), mass with respect to the mass of the unit DPD fluid particle, and energy with respect to kT . The non-dimensionalised value of solid radius is an important parameter as it sets the value of the r_c , which is indicative of the length scales being resolved and the level of coarse-graining in the system. The higher the value of this parameter, the lower the value of r_c , which means smaller and smaller scales are being probed, albeit at the expense of more computations and, possibly, redundancy. As is well known, in these systems a large span of length scales exists and the core idea behind mesoscopic simulations like DPD is to consider only the scales that are consequential to the bulk rheology of the system, which is the focus of attention here. On the other hand, too small a value of non-dimensionalised solid radius means shorter scales are less accurately resolved. Therefore, the choice of non-dimensionalised solid radius is an important call. As noted in Padding and Louis [15], a value more than two ensures satisfactory resolution of relevant hydrodynamic scales. Based on this, a solid particle radius of four was

used and accordingly a $20 \times 20 \times 20$ system-size was chosen. These choices provided an optimal balance between accuracy and computational load. The value of F_0 in Equation (1) in a non-dimensionalised unit is 60 for this system; Debye length ($1/\kappa$) has a non-dimensionalised value of 0.1.

Peclet number (Pe) and Reynolds number (Re) are the two most relevant (and independent) non-dimensional parameters in these suspensions [9]. For micron-sized particles and reasonable shear rates ($10\text{--}1000\text{ s}^{-1}$), $Re \ll 1$, in which case the reduced viscosity can be considered to be a sole function of Pe as elaborated in Stickel and Powell [9].

Just like the length scales, it is important that pertinent time scales are resolved by the computational scheme; for in these system there exist time scales that span several orders of magnitude [15], resolving all of which is obviously impossible and needless. The fact that Peclet number is the most important parameter for these sheared systems provides us with a convenient way to ascertain the relevant time scale and accordingly non-dimensionalise the shear rate. To do so, Peclet number ($= 6\pi\mu a^3 \gamma_r / kT$) for the system is first calculated using the real material properties and experimental shear rates. The viscosity of solvent (μ) is 0.001 Pa, the solid particle radius (a) is $0.475\text{ }\mu\text{m}$ and kT corresponding to $T = 300\text{ K}$ is $4\text{e-}21\text{ J}$. The shear rate (γ_r) is varied from 10 to 100 s^{-1} in the experiments. This value was then equated with the Peclet number calculated using the same parameters in DPD units, thus giving a relationship between the actual shear rate, the non-dimensionalised shear rate, material properties, and non-dimensionalised solid particle radius as shown below in Equation (2):

$$\gamma_r = Ma_n \gamma_{nd}, \quad (2)$$

where γ_r is the shear rate in s^{-1} used in the experiments, a_n is the non-dimensionalised solid particle radius, M encompasses material properties and parameters such as the viscosity of the solvent, size of the solid particles, temperature, etc., and γ_{nd} is the non-dimensionalised shear rate. This equation shows that in the regime of low Reynolds number the rheology depends on a combination of the shear rate (γ_{nd}) and solid particle size (a). Hence, computationally, there is some elbow-room to manoeuvre within these parameters, which is very desirable in computational modelling. Considering the fact that shear rate has the unit of inverse of time, the factor Ma_n^3 in Equation (2) therefore is indicative of the time-scale of the sheared system.

Using the properties, principles and set-up described above, computations were carried out for the mono-disperse cases of 10 and 30% solid loading by volume. The comparison with experiments is shown in Figure 2. As can be seen, the computed reduced viscosities

Table 1. A summary of forces used in the DPD formulation for the non-freezing case.

Summary of pair-wise DPD forces between particles i and j [1,2].
$F_{ij}^c = a_{ij}(1 - r_{ij})\hat{e}_{ij}$; $F_{ij}^D = -\gamma\omega_D(r_{ij})[\hat{e}_{ij} \cdot v_{ij}]\hat{e}_{ij}$;
$F_{ij}^R = \sigma\omega_R(r_{ij})\hat{e}_{ij}\xi_{ij}$
$k_B T = \sigma^2/2\gamma$; $\omega_D = (\omega_R)^2$; $v_{ij} = v_i - v_j$
Between two solid particles:
Equation (1) is used for F_{ij}^c ; $\gamma = 0$
Between a solid particle and fluid particle:
$a_{ij} = 12.5$; $\gamma = 5.6$
Between fluid particles:
$a_{ij} = 25$; $\gamma = 5.6$

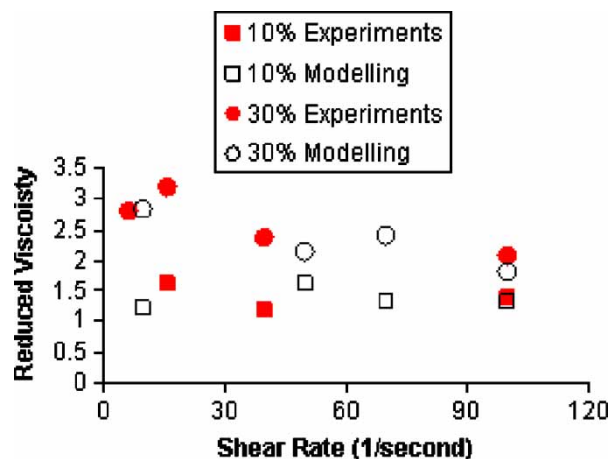


Figure 2. Comparison for the mono-disperse PS suspensions. Experimental values are represented by filled symbols.

compare well with the experiments. For the dilute case of 10% the suspension-reduced viscosities show little dependence on shear rate and the values compare favourably with Batchelor's second order correction to Einstein's formula for dilute suspensions [9] (<10% solid loading):

$$\eta_r \approx 1 + 2.5\varphi + 7.6\varphi^2 + O(\varphi^3), \quad (3)$$

where φ is the solid loading value. At low shear-rates a difference of around 20% is seen between the experimental and numerical data, whereas at higher shear the difference is negligible. We attribute this discrepancy primarily to the experimental technique involving the parallel-plate viscometer. At low shear-rates, for these dilute, lowly viscous materials the low values of torque signal contribute to some errors. The fact that at this dilution a Newtonian-type behaviour is predicted by the model (based on particle-level material properties) in close agreement with experiments and reported findings [9] lends strong credence to the approach.

For the 30% case, an overall shear thinning behaviour is predicted by the computations. This is in line with the behaviour of a non-dilute hard sphere model [8,9]. As the shear rate increases the shear forces overwhelm the equilibrium-restoring Brownian fluctuations and other electrostatic interactions and make the suspension more responsive to shear, thereby reducing the effective viscosity. This effect is seen here, both in experiments and in modelling. The favourable comparison also validates our approach of using solid particles (up to a certain size) as individual computational entities, entailing substantial savings in computations.

As mentioned earlier, in the hard sphere model appropriately used here, the hydrodynamic forces

predominantly dictate the behaviour of the system. However, as noted in van der Vorst *et al.* [16], it is worth mentioning that for non-dilute suspensions containing strongly interacting PS spheres in solvents with excess electrolyte concentration the non-hydrodynamic (electrostatic) interactions can overwhelm the hydrodynamic interactions and dictate the rheology of the system, particularly at low shear rates. This situation, however, does not apply to the system studied here.

4. The freezing approach

The basic aspects of the freezing approach for solid particles are explained in [2] and references cited there. In what follows some finer details that were found to be important in implementing this approach are explained first and then comparisons with experiments are reported.

4.1 Freezing approach

In the freezing approach unit DPD particles are frozen together into a larger particle of desired shape and size. In the collision and propagation steps of the transient simulation, care is taken so that the frozen particles always move together as one rigid entity without relative motion [2]. Each of the constituent frozen DPD particles then interacts with other particles in a normal fashion with DPD force-fields. This approach ensures that the shape and size aspects of the solid particles, that have profound effects on the hydrodynamics of the system, are captured and accounted for. In Figure 3, for purely demonstration purposes, the efficacy of the freezing technique is shown; a hypothetical suspension of cubical and spherical particles was generated and a snapshot of only the 'frozen' solid particles is shown to reiterate that particle shapes are maintained by the technique.

This representation should also enforce the impenetrability condition, which, if not addressed, may have undesired consequences on the dynamics of the system. DPD interactions are soft and therefore allow the fluid particles to hop into the solid, which is clearly unphysical. Barring the availability of force-fields that can ensure impenetrability in a natural way, the only option is to devise methods to minimise the instances of penetration and to mitigate the adverse consequences of the *ad hoc* methods. This was the approach adopted here. The translational motion of the composite solid particles is rigorously resolved but the rotational motion about their own axes is not explicitly calculated. The latter is not expected to have any noticeable effect on macroscopic quantities like viscosity since the solid

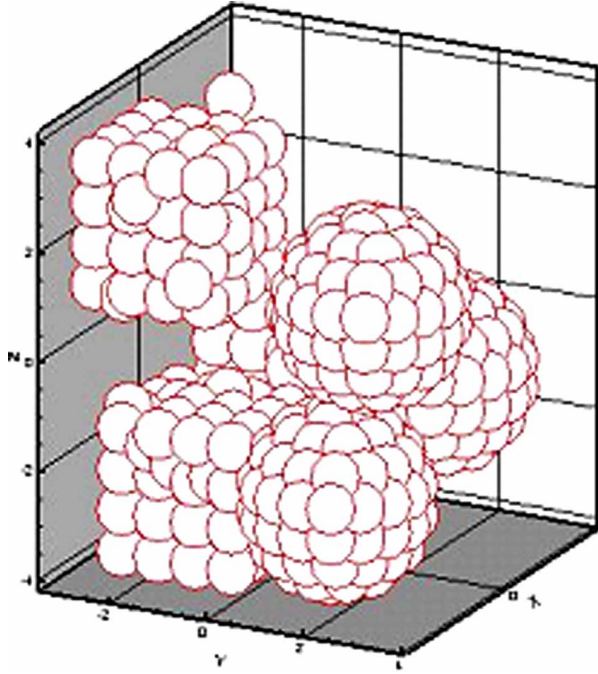


Figure 3. A snapshot of solid particles of cubical and spherical shapes in a hypothetical suspension to demonstrate the ability of the freezing technique to reproduce exact shapes.

particles considered here are of symmetric shapes and the imposed velocity field (using a Couette flow set-up) is planar. For more complex shapes and non-planar velocity fields it would be necessary to include these additional factors.

In the traditional implementation of the freezing algorithm in DPD, all particles, belonging to both fluid and solid phases, are treated alike as possessing finite mass but no volume, i.e. they are like points. One way of mitigating the problem of penetration is to assign a finite volume to the DPD particles that are frozen into solids. This way the composite solid particle will acquire an exclusion volume.

There are many ways of ensuring a finite volume of selected particles. One way is to alter the inter-particle conservative force so that the force at distances at which the finite volume is intruded upon becomes finitely high. To elaborate, as noted in references [2,5] the conservative force F^c between (point) particles labelled i and j in standard DPD is typically:

$$F^c = a_{ij}(1 - r), \quad (4)$$

a_{ij} is specific to the interaction pair and r is the inter-particle distance. According to this expression, the conservative force becomes maximum, equal to a_{ij} , when $r = 0$. If one of the particles, say the particle labelled i , is the frozen particle (and particle j is the fluid particle) then the expression can be modified as an attempt to give

particle i an excluded volume of the size of unit DPD particle, as

$$F^c = \frac{a_{ij}}{1 - r_f}(1 - r), \quad (5)$$

where r_f is the radius of the unit DPD particle that can be calculated from volume and particle density values. What Equation (5) says is that the maximum value of Equation (4), a_{ij} , is reached at $r = r_f$, much earlier than $r = 0$ in Equation (4). This implies that particle i tries to maintain an excluded volume of radius r_f , and that a much larger force than the nominal maximum is need to penetrate it by other particles.

Another modification that was found to be of immense benefit pertained to the bounce-back condition. The traditional bounce-back condition, as reported in the literature [17], places the penetrated fluid particle back into the fluid phase with the relative velocity between the fluid and solid particles reversed. Clearly local conservation laws are violated (as momentum is not strictly conserved) and, not surprisingly, if too many of these moves are made spurious oscillations in local temperature and density result. This can lead to an incorrect prediction of macroscopic phenomena, particularly for systems with high solid loading.

One way to remedy this is to try to conserve momentum in the bounce-back process by treating it as an elastic collision between the DPD fluid particle and the much larger rigid solid particle. In this case, the bounced-back velocity of the fluid particle would be [10,11]:

$$V' = V - 2 \frac{m_s V_{fs}}{m + m_s} \vec{n}. \quad (6)$$

In the above expression V' and V are velocities of the fluid particle after and before the collision, $V_{fs} = V - V_s$ where V_s is the rigid solid particle velocity, m_s is the mass of the solid particle, m is the mass of the DPD fluid particle and \vec{n} is the unit vector drawn from the fluid particle to the centre of the rigid solid particle.

Numerical experiments with the above-mentioned modifications – assigning a finite volume to frozen DPD particles and treating bounce-back as an elastic collision process – showed good improvement over the traditional bounce-back condition data. The main indicators in this assessment were the number of fluid particles penetrating the solid particles during the course of the simulation, and the behaviour of DPD thermostat in maintaining constant temperature. In the validation cases presented below these modifications were used.

4.2 Validation with standard problems

The first case considered for testing the new freezing mechanism was the case of 30% mono-disperse spheres ($0.95\ \mu\text{m}$ diameter) for which experiments were performed and the non-freezing approach was described earlier. Using the freezing approach for solid particles, the same case was simulated and compared with the validated non-freezing approach as shown in Figure 4. The reduced viscosity values are close and both the approaches show a similar overall trend – the expected shear thinning behaviour at moderately high shear rates. The maximum discrepancy between them is around 20% for which we believe the freezing approach is blame-worthy. As mentioned earlier, despite improvements in DPD force-fields and the bounce-back condition, particles still manage to penetrate the ‘frozen’ solid entity, although at a much lesser rate. These penetrations (which are spurious) and the subsequent remedial steps might have a mild effect on the calculated viscosity. However, as seen in Figure 4, the viscosities are in the same neighbourhood as that of the experiments and they

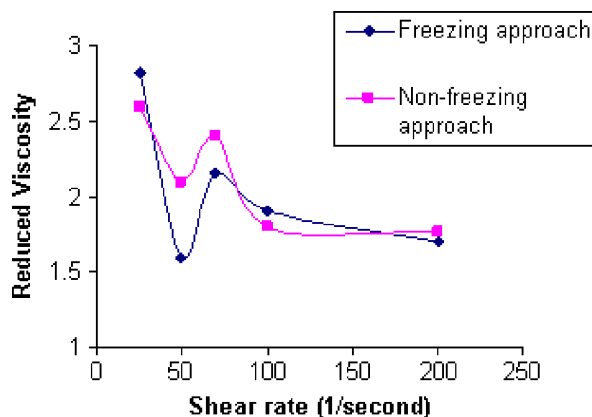


Figure 4. Comparison between the freezing approach and the non-freezing approach for the case of 30% mono-disperse suspension of spheres.

show a similar trend. With improvements in the freezing technique it is expected that these differences can be further mitigated. This comparison also validates the non-freezing approach in which solid particles of up to

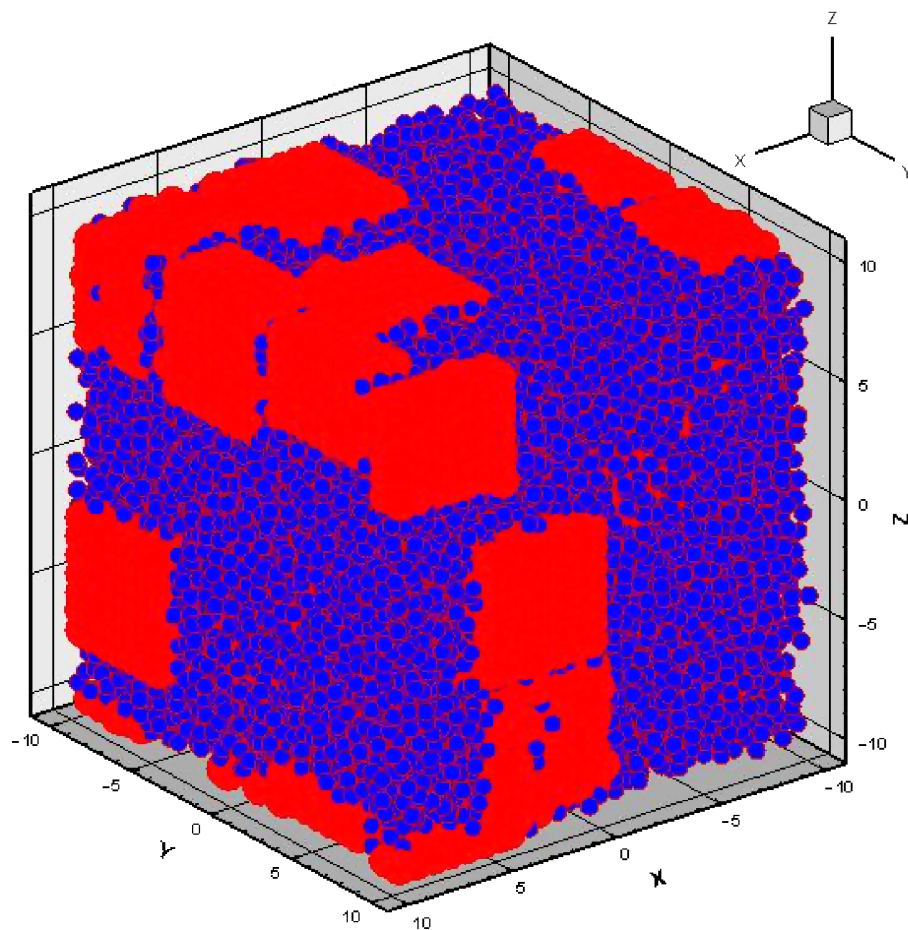


Figure 5. A snapshot showing the ‘frozen’ cubical particles in a sea of fluid particles during the course of the simulation. The blue particles are fluid particles and the red particles comprise the solid (cubic) particles.

micron size could be treated as unit computational entities with colloidal interactions. The non-freezing approach, it should be noted, saves computations as the number of computational particles in the system is smaller, and therefore should be utilised whenever possible.

Next, to test the validity of the freezing mechanism for non-spherical particles, a 30% suspension of mono-disperse cubic particles was simulated under the same shearing conditions. For consistency, the edge length of the cube was chosen to give the same surface area as the sphere in the above simulations. The simulations were performed in the same sized domain of $20 \times 20 \times 20$. A snapshot of the simulation is shown in Figure 5 in which the frozen cubical particles in a sea of fluid particles are shown. The reduced viscosities are shown in Figure 6 with a comparison of the 30% suspension of mono-disperse spherical particles (the case simulated above using the freezing technique). The suspension of cubes shows consistently higher viscosities than the suspension of spheres, particularly at low shear rates. This is to be expected, as the overall drag on the surface of a cube is more than that of a similar area of a sphere in the same flow conditions [9]. Also as expected, a prominent shear thinning behaviour is seen for the suspension of cubes. Although no experimental data is available for the suspension of cubes, we believe that the qualitative trend makes perfect sense, particularly in the low-shear regime. At high shear rates the difference in viscosities seems to be decreasing. Without experimental evidence, perhaps the best physical explanation that can be put forth is that at higher shear rates the effect of shape-related factors is diminished in relation to other factors that affect viscosity such as velocity magnitudes, higher dissipation rates, etc. Further work on this issue is underway.

4.3 Future work

As mentioned before, in the practical use of DPD for suspension rheology, computational expense is a serious issue. Computational load is directly related

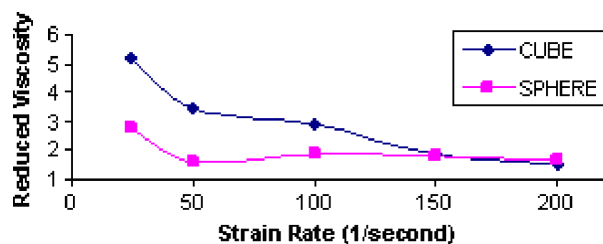


Figure 6. Comparison between 30% suspensions of cube and spheres.

to the number of particles in the formulation, with the freezing approach increasing the number of particles substantially. This can be gauged in the simulations presented here, with one frozen solid particle typically comprising of 500–1000 U DPD (computational) particles. One way of reducing the number of particles is by representing larger solid particles as ‘frozen’ aggregates of spherical colloids rather than the contemporary method of representing them as aggregates of unit fluid particles, which are much smaller than colloids. Since using the colloidal interaction as a conservative force in the DPD framework is valid, this approach is certainly noteworthy and is being pursued.

5. Conclusions

In this article, the traditional DPD methodology [2,5] was further expanded to yield a computationally efficient methodology for non-dilute suspensions. Specific experiments were performed with tailored suspension and employing a DPD force-field, derived using material properties, a good comparison with numerical calculations was obtained. This demonstrates that DPD can be used as a predictive, quantitative tool for rheology rather than just a generic, qualitative technique. The freezing approach for rigid solid particles was further refined for accuracy, and a new cost-saving direction was suggested. The approach of representing spherical solid particles of up to a micron in size as unit computational particles in DPD was presented in detail and validated. This approach can entail significant savings in computational costs.

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