Numerical Investigations On the Compressibility of a DPD Fluid

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Abstract

The compressibility of a dissipative particle dynamics (DPD) fluid is studied numerically through several newly developed test models, where both the density and the divergence of the velocity field are considered. In the case of zero conservative force, the DPD fluid turns out to be compressible. Effects of the compressibility are observed to be reduced as the particle mass is chosen to be smaller and the system temperature to be higher. In the case of non-zero conservative force, the condition of constant density and divergence-free of velocity can be approximately achieved at large values of the repulsion parameter (i.e., weakly compressible flow). Furthermore, the speed of sound and local Mach number are computed and found to be in good agreement with the theoretical estimation.

Keywords: Dissipative Particle Dynamics, Compressibility, Bulk viscosity, Speed of sound

1. Introduction

The dissipative particle dynamics (DPD) method, first introduced by Hoogerbrugge and Koelman [1], is meant to be a mesoscaled simulation technique yielding correct hydrodynamic behaviors and has its basis in statistical mechanics [2, 3]. Originally, each DPD particle is regarded as a cluster of molecules, undergoing a soft potential with respect to others and the method was conceived as an improvement over the molecular dynamics (MD) with high computational efficiency. The motions of DPD particles are governed by Newtonian second law in a continuous space, and hence, it can avoid the problem faced by lattice-gas automata (LGA) [4] (absence of isotropy and Galilean invariance). Under some restrictions on the interaction potential, the DPD method conserves both the number of particles (mass) and also the total momentum of the system which can overcomes some drawbacks of the Brownian Dynamics Simulation (BDS) method [5]. Meanwhile, both the flow kinematics and the stress tensor can be found as parts of the solution procedure.

Based on the features mentioned above, the DPD method should be an attractive and powerful tool in simulating flow problems, and it was in fact widely used in the last two decades - it can be indeed regarded as a particle-based method for solving continuum flow problems of complex-structure fluids, owing to its conservation of mass and momentum. Due to the nature of Lagrangian description of this particle-based approach, complex flow structures can be handled by DPD in a simple manner. For instance, for flow around cylinder or sphere, the solid phase can be composed by a set of frozen DPD particles on the solid surface, or its interior [1, 6, 7] or even a single DPD particle with different parameters to distinguish itself from the surrounding solvent DPD particles [8]. By connecting certain DPD particles to form chains, suspensions of polymer or DNA molecules can be and have been simulated [9–12]. Immiscible droplets suspended in another solvent have been also modeled by two different sets of DPD particles with a larger repulsion force specified on the interface [13, 14]. In addition, red blood cell (RBC) can be modeled by connecting the surface particles of the cell [15].

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DPD method is certainly a promising numerical approach in simulating complex fluid phenomena. However, as a particle-based method, it may suffer from the compressibility effect as the original smooth particle hydrodynamics (SPH), for which much effort have been made to control the fluid compressibility [16, 17]. To our knowledge, the compressibility of DPD fluids was seldom investigated in the past, and was mentioned only in passing in few works. Kim and Phillips [6] first reported that the drag force acting on a sphere cannot be predicted accurately by DPD when the Reynolds number is in excess of 100, and they attributed the reason to the compressibility of DPD fluid. For a high Reynolds number flow, a high Mach number is also resulted. Van de Meent et al. [18] studied the coherent structures of the transition to turbulence in compressible shear flows with DPD. In their work, they first obtained the speed of sound in a DPD fluid by measuring the speed of propagation of a density pulse. However, the details were not reported in their paper. In hydrodynamics, the fluid is usually assumed incompressible so that both a constant density and a divergence-free velocity field are expected. In this paper, it is our intent to examine carefully and systematically the compressibility of a DPD fluid, and both the density and the velocity divergence are investigated numerically. One objective is to provide information on compressibility of DPD fluid that others may find it useful in further applications. In the following sections, the DPD method will be firstly reviewed. Then, two different numerical models are discussed and the corresponding numerical results concerning the compressibility of the DPD fluid as well as the speed of sound in the DPD fluid will be presented. Finally, some remarks will be given.

2. DPD methods

2.1. Overview

For the standard DPD method, the motion of DPD particles is governed by Newton second law of motion. For a simple DPD particle $i$,

$$\frac{dr_i}{dt} = v_i, \quad m \frac{dv_i}{dt} = f_i + F^e,$$  

(1)

where $r_i$ and $v_i$ are the position and velocity vectors of particle $i$. We assume all the DPD particles have the same value of mass $m$. $f_i$ is the inter-particle force exerted by all the other particles and $F^e$ is the external force exerting on particle $i$. In the framework of Español and Warren [2], the inter-particle force $f_i$ contains three parts: a conservative force, a dissipative force and a random force, all are pairwise,

$$f_i = \sum_{j \neq i} \left( F^C_{ij} + F^D_{ij} + F^R_{ij} \right).$$

(2)

Here, the sum runs over all other particles within a certain cutoff radius $r_C$, which is usually taken as unity ($r_C = 1$), but it can be set at any value and can take on different values for different types of forces. In the DPD algorithm developed by Groot and Warren [19], the conservative force $F^C_{ij}$ is a soft repulsion acting along the line of centers and is given by,

$$F^C_{ij} = \begin{cases} a_{ij}(1 - r_{ij}) \hat{r}_{ij} , & r_{ij} < 1, \\ 0 , & r_{ij} \geq 1, \end{cases}$$

(3)

where $a_{ij}$ is the maximum repulsion between particle $i$ and particle $j$, and $r_{ij} = r_i - r_j$, $r_{ij} = |r_{ij}|$, $\hat{r}_{ij} = r_{ij}/|r_{ij}|$. Here in this paper, we take the cutoff radius for the conservative force to be unity, i.e., the unit of length. The other two forces are dissipative force $F^D_{ij}$ and random force $F^R_{ij}$, and they are given by

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

(4)

and

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

(5)
respectively. Here, $\gamma$ and $\sigma$ are two coefficients characterizing the strength of dissipative force and random force, $w^D(r)$ and $w^R(r)$ are the weight functions for these two forces vanishing for $r \geq r_C$, $\mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j$ is the relative velocity and $\theta_{ij}$ is a white noise with the properties

$$\langle \theta_{ij}(t) \rangle = 0$$

and

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

where $\langle \cdots \rangle$ denotes an ensemble average with respect to its own distribution function.

In order to satisfy the balance condition (fluctuation-dissipative theorem), Español and Warren [2] showed that one of the two weight functions in Eq.(4) and Eq.(5) can be chosen arbitrarily and then the other is determined by,

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

where $k_BT$ is the Boltzmann temperature of the system (a measure of the fluctuating kinetic energy of the system). In this paper, we adopt a generalized form for the dissipative weight function proposed in [12]:

$$w^D(r) = [w^R(r)]^2 = \begin{cases} \left(1 - r/r_C\right)^s, & r_{ij} < r_C, \\ 0, & r_{ij} \geq r_C, \end{cases}$$

where $r_C$ and $s$ are the cutoff radius and exponent, respectively. In the conventional DPD system as introduced by Groot and Warren [19], these two parameters are set as $r_C = 1.0$ and $s = 2$, while in order to improve the dynamic response and increase the Schmidt number of the DPD system, Fan et al. [12] preferred $s = 1/2$ and $1.0 \leq r_C \leq 1.5$. Throughout this paper, we employ $r_C = 1.0$ and $s = 1/2$.

2.2. Simulation procedure

In our numerical simulation, initially the particles are located the face-centered cubic (FCC) lattices sites. The size of the cubic lattices are fixed to be unit which means the side length of all the lattices is equal to 1 and the corresponding number density is 4. The initial velocities of all the particles are set randomly according to the system temperature $k_BT$. To solve Eq.(1), the velocity-Verlet algorithm [19] is employed here,

$$\begin{align*}
\mathbf{r}_i(t + \Delta t) &= \mathbf{r}_i(t) + \Delta t\mathbf{v}_i(t) + \frac{1}{2}\Delta t^2\ddot{\mathbf{v}}_i(t), \\
\dot{\mathbf{v}}_i(t + \Delta t) &= \dot{\mathbf{v}}_i(t) + \lambda\Delta t\ddot{\mathbf{v}}_i(t), \\
\ddot{\mathbf{v}}_i(t + \Delta t) &= \ddot{\mathbf{v}}_i(t) + \dddot{\mathbf{v}}_i(t + \Delta t),
\end{align*}$$

where $\dddot{\mathbf{v}}_i(t)$ is the acceleration of the particle $i$ at the instant $t$, $\dot{\mathbf{v}}_i(t + \Delta t)$ denotes the prediction of the velocity of the particle at the instant $t + \Delta t$, and $\lambda$ is an empirically introduced parameter to account for some additional effects of the stochastic interactions. Groot and Warren [19] found the optimum value of $\lambda$ is 0.65 and in their paper the time step can be increased to 0.06 without loss of temperature control in simulating an equilibrium system with density $\rho = 3$ and $\sigma = 3$. In addition, since the initial FCC distribution of the particles do not represent a thermodynamic equilibrium state, at the beginning of the simulation the particle are allowed to move with periodic boundary conditions along three directions until a thermodynamic equilibrium state is reached.

Periodic boundary conditions along all the three directions are used in the current simulation, which automatically satisfy no-slip condition on the solid wall [11, 20–24].

The stress tensor is calculated using the Irving-Kirkwood model [25]. The contribution from each particle on the stress tensor component $S_{\alpha\beta}$ can be divided into two parts:

$$S_{\alpha\beta} = -\frac{1}{V} \left\langle \sum_i N_p m u_{i\alpha} u_{i\beta} + \sum_i \sum_{j>i} N_p \sum_{l=1}^N r_{ij\alpha} F_{ij\beta} \right\rangle,$$
where, \( N_p \) is the number of particles, \( u_{\alpha i} \) and \( u_{\beta i} \) are the peculiar velocity components of particle \( i \), defined by \( u_{\alpha i} = v_{\alpha i} - \bar{v}_\alpha(x) \) (\( v_{\alpha i} \) is the velocity component of particle \( i \) and \( \bar{v}_\alpha(x) \) the stream velocity at position \( x \)), and \( F_{ij} \) is the inter-particle force component between particle \( i \) and particle \( j \).

3. Compressibility of DPD fluid

The general form for a Newtonian stress tensor can be written as [26]:

\[
S(r, t) = -pI + \zeta \nabla \cdot uI + \eta(\nabla u + \nabla u^T - \frac{2}{3} \nabla \cdot uI),
\]

where \( p \) is the hydrostatic pressure, \( \eta \) the shear viscosity, \( \zeta \) the bulk viscosity and \( I \) the unit tensor. Based on this, an equivalent “Poisson ratio” \( \nu \) of the material, analogous to that of a linear elastic material, can be derived [27]

\[
\nu = \frac{\zeta - \frac{2}{3}\eta}{2(\zeta + \frac{4}{3}\eta)}.
\]

For different kinds of materials, the values of Poisson ratio range as \(-1 \leq \nu \leq 1/2 \) and the limit \( \nu = 1/2 \) corresponds to an incompressible material. Recall that the Poisson ratio is the lateral contraction ratio of a bar of a linear elastic material under an extension. For a DPD fluid, Marsh [3] first made some theoretical estimations (ignoring the contribution of conservative force \( F^c_{ij} \)) on both the shear viscosity and the bulk viscosity which we will be reviewed, in addition to a comparison between water and a DPD fluid. In the section 3.2, numerical experiments are made to investigate the compressibility of a DPD fluid, the density distributions and the divergence of velocity fields are also analyzed to assess the effects of the conservative force.

3.1. Theoretical Estimation

Marsh [3], with the help of Chapman-Enskog expansion, derived an approximate evolution equation for the single particle distribution function of the DPD system neglecting the conservative force \( F^c_{ij} = 0 \), and the kinetic theory was applied to extract the transport coefficients (shear viscosity \( \eta \) and bulk viscosity \( \zeta \)) of the DPD fluid:

\[
\eta = \eta_D + \eta_K = \frac{\gamma n^2 [R^2 w_D]_R}{2d(d + 2)} + \frac{dnk_BT_0}{2\gamma [w_D]_R},
\]

\[
\zeta = \zeta_D + \zeta_K = \frac{\gamma n^2 [R^2 w_D]_R}{2d^2} + \frac{mkn_BT_0}{\gamma [w_D]_R}.
\]

Here, \( n \) is the particle number density (the local mass density \( \rho \) of the DPD fluid is simply \( \rho = nm \) ), \( d \) the dimension of the system and is set to 3 in the paper. Both the shear viscosity and bulk viscosity have two contributions, from the dissipative part denoted by the subscript \( D \) and from the kinetic part denoted by the subscript \( K \), corresponding to the contributions from dissipative and random forces, respectively. The short-hand notation \([\cdots]_R \) in Eq.(12) and Eq.(13) represents the integral over space \( [f(R, v, t)]_R = \int dR f(R, v, t) \). Therefore, the weighting function defined in Eq.(7) can be derived as,

\[
[w_D]_R = 4\pi r_C^3 \left( \frac{1}{1+s} - \frac{2}{2+s} + \frac{1}{3+s} \right),
\]

\[
[R^2 w_D]_R = 4\pi r_C^5 \left( \frac{1}{1+s} - \frac{4}{2+s} + \frac{6}{3+s} - \frac{4}{4+s} + \frac{1}{5+s} \right),
\]

where, \( s \) is the exponent in Eq.(7).
Table 1: Comparison of viscosities and Poisson ratios between water at 25°C and DPD fluid.

<table>
<thead>
<tr>
<th></th>
<th>Water(25°C) [28]</th>
<th>DPD fluid</th>
</tr>
</thead>
<tbody>
<tr>
<td>Viscosity (η)</td>
<td>0.88 mPa·s</td>
<td>2.40</td>
</tr>
<tr>
<td>Viscosity (ζ)</td>
<td>2.47 mPa·s</td>
<td>3.83</td>
</tr>
<tr>
<td>Poisson ratio (ν)</td>
<td>0.34</td>
<td>0.24</td>
</tr>
</tbody>
</table>

With these estimates, a comparison of these properties between water (25°C) [28] and our DPD fluid is shown in Table 1. The parameters of DPD fluid here are set as: \( m = 1.0, k_B T = 1.0, r_C = 1.0, s = 1/2 \) and \( γ = 4.5 \).

Obviously, for both water and the DPD fluid, the Poisson ratios of them are less than 0.5 and hence cannot be treated as absolutely incompressible. However, the speed of sound in water at 25°C is very high, at nearly 1500 m/s, its time scale corresponding to sound wave traveling in the water is very small compared with the time scale for the motion of bulk flow and a lower Mach number results. In this situation, water can be treated as incompressible. While for our DPD fluid, the time scale corresponding to its speed of sound may not be as small, compared to the time scale of particle motion, which results in a significant compressibility effect.

3.2. Numerical Experiments

Here in this section, the compressibility of a DPD fluid will be investigated numerically. Simple shear flow may not be a good vehicle to explore compressibility effects; we need a flow field in which a non-zero divergence of velocity may be promoted. Similar to the experiment for measuring Poisson ratio of a linear elastic material, we intend to stretch the DPD fluid in an elongational flow. However, in this situation, the boundary conditions may be not so straightforward for this particle-based simulation method in which periodic boundary conditions are mainly used. To overcome this, a new computational model shown in Fig. 1 is constructed.

![Figure 1: Sketch of model for elongational flow.](image)

In the computational domain as shown, we focus on a smaller box, placed at the center of the computational domain. Full periodic boundary conditions are prescribed for the particles on the surfaces of the computational domain, preserving mass globally. For the smaller box, particles on the surfaces normal to the \( x \)-direction are prescribed a \( x \)-component velocity, \( -V_x \) and \( V_x \) on the surface facing the negative and positive \( x \)-directions, respectively (refer to Fig. 1), corresponding to a uni-axial elongational flow. We expect particles on the lateral sides of the smaller box (dashed arrows in Fig. 1) to move into the smaller box, through its lateral sides, thus mimicking a uni-axial elongational flow.
Furthermore, we also vary the parameters, such as $m$, to be 0.

For four cases are close to each other at around 0.

3.2.1. DPD fluid without conservative force ($F^C = 0$)

In this simulation, we monitor the particles’ velocities when they cross through the lateral four surfaces in responded to $V_x = 1$. The lateral velocities of the particles entering the smaller box are found to be reasonably constants and are the same on the four lateral surfaces on average. We denote by $V_m$ the mean velocity of particles entering through all the four lateral surfaces. Its independence of domain size and time step are first verified. Table 2 gives some verification results for $V_m$ for four verification cases. The results for four cases are close to each other at around 0.33.

In order to obtain the local variables including velocity vectors and stress tensor, we divide the whole domain into bins and the flow properties are calculated by averaging over all sampled data in each bin. One typical flow field is shown in Fig. 2. The fluid flows out of the smaller box at $x$–direction, four rotational flow patterns are formed at the corners of the smaller box and then the fluid enters into the box at both $y$–direction and $z$–direction. In the plane of symmetry, our flow pattern resembles that of a four-roller mill, a device used to generate an approximate planar elongational flow at its center [29, 30]. In addition, as shown in Fig.2(a), the locations of the blue bars are corresponding with the surfaces of the small box where a prescribed velocity is assigned to the local particles, and an elongational flow is generated inside the small box. Since a prescribed velocity is assigned to the particles, their random velocities are ignored and zero temperature zones result. Since they are relative narrow zones, their effects on the overall region are not significant, and the temperature are uniformly distributed in everywhere else.

Table 2: Mean velocities of monitored surfaces of DPD fluid with $m = 1.0$ and $k_B T = 1.0$.

<table>
<thead>
<tr>
<th>$dt$</th>
<th>$(X,Y,Z)$</th>
<th>$V_x$</th>
<th>$V_m$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.005</td>
<td>(40,40,40)</td>
<td>1.0</td>
<td>0.321</td>
</tr>
<tr>
<td>0.010</td>
<td>(40,40,40)</td>
<td>1.0</td>
<td>0.325</td>
</tr>
<tr>
<td>0.005</td>
<td>(60,60,60)</td>
<td>1.0</td>
<td>0.328</td>
</tr>
<tr>
<td>0.010</td>
<td>(60,60,60)</td>
<td>1.0</td>
<td>0.328</td>
</tr>
</tbody>
</table>

For an incompressible fluid, the ratio of the entered velocity $V_m$ to the prescribed velocity $V_x$ is expected to be 0.5, which implies a zero velocity divergence. However, as shown in Table 2, the ratio is lower than 0.5, indicating of the compressibility character of the DPD fluid with the present parameters selection. Furthermore, we also vary the parameters, such as $V_x$, particle mass $m$ and system temperature $k_B T$, and monitor $V_m$. The results are shown in Tables 3–5. It is clear that the ratio $V_m/V_x$ increases toward 0.5 with decreasing $V_x$ or the particle mass, or when the system temperature increase. Specifically, when the particle mass equals to 0.2, $V_m$ is closed to 0.5 and the fluid might be considered incompressible. Here, we did not reduce the particle mass further, since a different integrating scheme may be needed for such a stiff stochastic system [31]. It is to be noted that lowering $V_x$ or $m$ effectively decreasing both the Reynolds number and the Mach number (to be demonstrated later), thus promoting incompressible flows.

We construct a series of virtual cubes which are centered at the smaller box with side length equal to $l_x$ to probe the flow properties inside each of the cubes. Figure 3 and Figure 4 give the mean number density and local temperature versus different side length cubes for different cases. Obviously, a change in the mean density inside each cube implies a non-uniform density distribution. On the other hand, the temperature remains almost constant for all cases we considered, indicating that our system obeys the balance condition well. For the case with $m = 0.2$ as shown in Fig.4, the density does not change much with the size of the
Figure 2: Velocity vectors and temperature contours on the central slices.

Table 3: Mean velocities of monitored surfaces for different $V_z$ with $m = 1.0$ and $k_B T = 1.0$.

<table>
<thead>
<tr>
<th>$V_z$</th>
<th>$V_m$</th>
<th>$V_m/V_z$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.50</td>
<td>0.242</td>
<td>0.484</td>
</tr>
<tr>
<td>0.75</td>
<td>0.289</td>
<td>0.385</td>
</tr>
<tr>
<td>1.00</td>
<td>0.328</td>
<td>0.328</td>
</tr>
<tr>
<td>2.00</td>
<td>0.380</td>
<td>0.190</td>
</tr>
</tbody>
</table>
Table 4: Mean velocities of monitored surfaces for different particle mass $m$ with $V_x = 1.0$ and $k_B T = 1.0$.

<table>
<thead>
<tr>
<th>$m$</th>
<th>$V_m$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.20</td>
<td>0.464</td>
</tr>
<tr>
<td>0.50</td>
<td>0.386</td>
</tr>
<tr>
<td>1.00</td>
<td>0.328</td>
</tr>
<tr>
<td>2.00</td>
<td>0.247</td>
</tr>
</tbody>
</table>

Table 5: Mean velocities of monitored surfaces for different temperature $k_B T$ with $V_x = 1.0$ and $m = 1.0$.

<table>
<thead>
<tr>
<th>$k_B T$</th>
<th>$V_m$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.10</td>
<td>0.131</td>
</tr>
<tr>
<td>0.50</td>
<td>0.250</td>
</tr>
<tr>
<td>1.00</td>
<td>0.328</td>
</tr>
<tr>
<td>2.00</td>
<td>0.407</td>
</tr>
</tbody>
</table>

cube, while for case with $k_B T = 0.1$, the density varied much more when compared with the other cases. The results are consistent with those presented in Tables 4 – 5, and it can be concluded that the DPD fluid under the current condition is indeed compressible for certain choices of parameters.

After confirming the compressibility of a DPD fluid, next we intend to measure the bulk viscosity of DPD fluid numerically. The bulk viscosity can be obtained by taking the trace of stress tensor of Eq.(10) in a straightforward manner, which was usually done in MD simulations [32, 33]. However, after a close inspection to Eq.(13), we found that the value of bulk viscosity is related to its local number density as well as temperature. In the present simulation, the number density can be non-uniform corresponding to the compressible nature of DPD fluid. Therefore, the bulk viscosity may not be uniform throughout the whole domain. In order to verify the theoretical estimation of Marsh [3], we construct the trace of stress tensor in two different ways, one corresponding to his theoretical estimation and the other, to our numerical simulation. In the manner after the theoretical estimation, we derive the trace of stress tensor $tr S_c$ from the constitutive relation of Eq.(10) and only the hydrostatic pressure and bulk viscosity terms provide contributions to the trace. As shown below, we average the trace of the stress inside the monitored cube:

$$tr S_c = \frac{1}{V} \sum_{i,j,k} tr S_c(i,j,k) = -3p + \sum_{i,j,k} \nabla \cdot \mathbf{v} + 3 \zeta(i,j,k) \nabla \cdot \mathbf{v}(i,j,k). \quad (16)$$

Here, $n(i,j,k)$, $k_B T(i,j,k)$ and $\nabla \cdot \mathbf{v}(i,j,k)$ are number density, temperature and divergence of velocity in each bin inside the monitored cube. $\zeta(i,j,k)$ is the bulk viscosity calculated from Eq.(13) with the local properties, such as number density, temperature in each bin.

In the manner of the numerical simulation, we derive the trace of stress tensor $tr S_k$ from the Irving-Kirkwood model in Eq.(9) and average it inside the monitored cube as:

$$tr S_k = \frac{1}{V} \sum_{i,j,k} tr S_k(i,j,k). \quad (17)$$

Here, $S(i,j,k)$ is the stress tensor of each bin inside the cube. Figures 5 – 6 give the comparisons of these two traces of stress tensors for different cases, with varying $V_x$, particle mass $m$ and system temperature $k_B T$. These two kinds of traces of stress tensors are close to each other inside the different sized cubes for different cases. Therefore, under the condition of $F_{ij} = 0$, the bulk viscosities of DPD fluid of the theoretical estimation of Marsh [3] and numerical simulation in this paper are consistent with each other, which incidentally also affirms the compressibility of DPD fluid.

3.2.2. DPD fluid with conservative force ($F^C \neq 0$)

We next consider the effects of conservative force. In the paper of Groot and Warren [19], they first derived a relationship between the repulsion parameter $a_{ij}$ in the conservative force and the compressibility of the system. By establishing the equation of state for DPD fluid, they recommended the following relation (for water-like fluids at room temperature 300K):

$$8$$
Figure 3: Mean temperature constant $k_B T$ and number density $n$ of center cubes with different side length $l_z$, the particle mass is set as $m = 1.0$. 

(a) $V_z = 1.0$

(b) $V_z = 0.5$
Figure 4: Mean temperature constant $k_B T$ and number density $n$ of center cubes with different side length $l_x$, the velocity $V_x$ is set to 1.0.

(a) $m = 0.2$

(b) $k_B T = 0.1$
Figure 5: Comparison of mean trace of stress tensor for cases with different $V_x$ and particle mass and temperature are set the same as $m = 1.0$ and $k_B T = 1.0$. 

(a) $V_x = 1.0$

(b) $V_x = 0.5$
Figure 6: Comparison of mean trace of stress tensor for cases with different particle mass $m$ and temperature $k_B T$, the prescribed velocity $V_x$ is set the same as $V_x = 1.0$. 

(a) $m = 0.2$

(b) $k_B T = 0.1$
\[
\frac{a_{ij}n}{k_B T} \approx 75.
\] (18)

According to the Eq. (18), if we set the number density equal to 4, particle mass equal 1, then the repulsion parameter \(a_{ij}\) should be 18.75 for \(k_B T = 1\). Here, we increase \(a_{ij}\) gradually from 0 in our numerical model. Figure 7 gives the monitored \(V_m\) with different \(a_{ij}\); the results show that \(V_m\) increases significantly when \(a_{ij}\) is larger than 0. When \(a_{ij} = 18.75\), \(V_m\) is about 0.46, and if we further increase \(a_{ij}\) to 40, \(V_m\) can be also increased but still lower than 0.5. In addition, if we set the particle mass equal to 0.2, \(V_m\) is about 0.6% from its incompressible value of 0.5. The mean number density in each monitor cube is also shown in Fig.8. For cases with large \(a_{ij}\), the number density inside of each cube is almost constant and close to 4. And if we set \(a_{ij}\) larger than the recommended value of 18.75, the DPD fluid is much closer to being incompressible.

![Figure 7: Ratios between mean monitored velocity \(V_m\) and prescribed velocity \(V_x\) for cases with different repulsive parameters \(a_{ij}\), the particle mass and temperature are fixed as \(m = 1.0\) and \(k_B T = 1.0\).](image)

We also calculated the divergences of the velocity field inside the smaller box by using the divergence theorem:

\[
\nabla \cdot \mathbf{v} = \frac{1}{V} \int_V \nabla \cdot \mathbf{v} dV = \frac{1}{V} \int_S \mathbf{v} \cdot \mathbf{n} ds = \frac{1}{V} \sum_{j=1}^{6} (\mathbf{v} \cdot \mathbf{n})_j S_j,
\] (19)

where, \(\mathbf{n}\) is the normal unit vector of the cubic surface and \(S_j\) is the area of each surface. The results are shown in Fig.9, and consistent with the results of Fig.8: the larger the \(a_{ij}\), the closer to incompressible is the outcome.

4. Speed of Sound and Mach number

As mentioned in previous section, the DPD fluid should be considered as a compressible fluid and hence, it is valuable to measure the speed of sound in DPD fluid and predict the local Mach number for certain flow pattern. The isothermal speed of sound \(c_s\) can be derived as \(c_s^2 = \frac{\partial p_0}{\partial \rho}\). If the characteristic velocity is \(V_c\) then the corresponding Mach number is \(Ma = \frac{V_c}{c_s}\). Groot and Warren [19] derived an approximation of the equation of state as:
Figure 8: Mean number densities inside the centered cubes with different side length $l_x$.

Figure 9: Mean divergences of velocity inside the centered cubes with different side length $l_x$. 
\[ p = n k_B T + \alpha a_{ij} n^2 \quad (\alpha = 0.101 \pm 0.001). \]  

Then, the square of speed of sound can be derived as,

\[ c_s^2 = \frac{k_B T}{m} + \frac{2n}{m} \alpha a_{ij} \quad (\alpha = 0.101 \pm 0.001). \]  

If we fix \( k_B T = 1.0, m = 1.0, n = 4 \) and \( a_{ij} = 18.75 \), then the speed of sound is about \( c_s \approx 4.0 \). In order to verify this numerically, we can use density perturbation to generate a sound wave. A numerical model shown in Fig.10 is used in this paper. DPD particles formed a cylinder with number a higher density equal to \( n_{in} = 6 \), initially is immersed in a box which is also formed by DPD particles but with a lower ambient number density of \( n_{out} = 4 \). A sound wave is generated which travels from the center to outside when the system is started up.

The local number density distributions on the \( x - z \) plane, captured at different times are shown in Fig.11. The phenomena of density transports are shown clearly in these contours. The speed of sound can be calculated by recording the position of wave crest at different moments. According to Eq.(21), the magnitude of sound speed is related to the local number density and temperature. However, in our numerical results, when the sound wave propagated outwards, the local number density is varying and a
little larger than 4. Hence, it is difficult to obtain the exact value of sound speed at certain number density. Under current parameters selection, the speed of sound is equal to 3.95 approximately which is close to the estimated value, Eq.(21), with a local number density around 4.3. The corresponding Mach number is about 0.25 (choosing the characteristic velocity equal to 1) and somewhat less than the critical value of 0.3 beyond which compressibility should be taken into account. An alternative way to promote the incompressibility of the fluid is to reduce the mass of the particles. According to Eq.(21), a smaller mass corresponds with a larger speed of sound and then a smaller Mach number is resulted.

5. Conclusions

The compressibility of a DPD fluid has been studied in this paper. As a promising particle-based numerical method, DPD has a wide application in simulating complex flow problems in many engineering fields. A numerical model with a specific boundary condition is employed in this paper to produce a flow field with non-zero divergence of velocity, without the boundary condition complications associated with the method.

Both the density and divergence of velocity field are investigated with this model. Under the condition studied in this paper, the DPD fluid is a compressible fluid when the conservative force is not considered. With a smaller particle mass or larger system temperature, the DPD fluid becomes more incompressible. Estimations of the bulk viscosity by Marsh [3] are verified with our numerical simulation as well - the numerical results are consistent with the theoretical estimation. For DPD fluid with conservative force, a larger repulsion parameter $a_{ij}$ can result in a weakly compressible fluid that both a constant density and divergence-free velocity are nearly satisfied. So although the fluid is compressible (with an equivalent Poisson ratio of around 0.3), we can promote incompressibility by a sensible choice of parameters - this is demonstrated by an inspection of the velocity field, and the density distribution to ensure of this.

The speed of sound in DPD fluid is also obtained by measuring the propagation speed of a density perturbation. If we set the characteristic velocity to be unit, the corresponding Mach number is close to 0.3 beyond which the compressible effect must be taken into account. To promote incompressibility, the Mach number should be reduced significantly below 0.3 - the best mean to achieve this may be to reduce the mass of the particles to obtain a near incompressible fluid.

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References

Figure 11: Evolution of DPD particle number density distributions with $m = 1.0$, $k_B T = 1.0$ and $a_{ij} = 18.75$. 

(a) $t = 0.4$

(b) $t = 1.0$

(c) $t = 1.6$