APPLICATION OF DISSIPATIVE PARTICLE DYNAMICS TO THE STUDY OF A RED BLOOD CELL IN SIMPLE SHEAR FLOW*

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The present work reports an attempt to apply the dissipative particle dynamics (DPD) method to study the dynamic behaviors of a red blood cell (RBC) in simple shear flow. The simulation system is discretized into four types of particles, namely wall particles, fluid particles, membrane particles and internal particles. The particle interaction is modeled by the DPD method, and the membrane particles are connected into a viscoelastic triangular network to represent the RBC membrane. As benchmarking tests, we simulate the deformation of a spherical capsule in shear flow and compare it with the past study, and also examine the effect of computational domain size. After that, we investigate the dynamics of a RBC in shear flow at different membrane shear and bending moduli. Our simulations reproduce the tank-treading, trembling and tumbling motions of the RBC at the shear modulus $E_s = 6, 60$ and $600 \mu\text{N/m}$, respectively. Moreover, we find that the RBC undergoes a trembling motion when its bending modulus is large enough, where the obvious stretching and smoothing of the RBC occur alternately in shape.

Keywords: Dissipative particle dynamics; tank-treading; trembling; tumbling.

1. Introduction

Dissipative particle dynamics (DPD) is a mesoscale stochastic simulation technique proposed by Hoogerbrugge and Koelman¹, which is considered to be a promising approach for complex fluid systems, such as multiphase flow² and suspensions³. However, it has not been widely applied to study the biological cells so far except in Karniadakis's Group⁴⁻⁸. The present work attempts to use the DPD method to study the dynamic behaviors of a red blood cell (RBC) in simple shear flow.

Dynamics behaviors of a cell (or capsule) in simple shear flow have been investigated by several numerical methods in past years, such as the boundary element method

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(BEM)^{9,10}, the lattice Boltzmann method (LBM)¹¹⁻¹³, the immersed boundary method (IBM)^{14,15}, the particle-based method¹⁶, the advected-field method¹⁷, and so on. These studies demonstrated that there are three dynamic modes of a cell (or capsule) in simple shear flow, namely the steady tank-treading, unsteady tumbling and transitional trembling modes, as shown in Fig. 1. In the tank-treading mode, the cell (or capsule) reaches a steady state with a stationary shape and fixed orientation, whereas its membrane rotates around the internal fluid continuously, like the tank treading. In the tumbling mode, the cell (or capsule) tumbles or flips in the original shape as a rigid body. In the trembling mode, however, the cell (or capsule) undergoes a shape deformation and orientation oscillation, and it is identified to be a transitional model between the first two modes.

Fig. 1. Different dynamic modes of a capsule in simple shear flow¹⁸, (a) the steady tank-treading, (b) the unsteady tumbling, and (c) the transitional trembling modes.

The present work focuses on the theoretical description, numerical implementation and validation of the DPD system coupled with a discrete cell model, and its application to study the dynamics of a RBC in simple shear flow. The simulation system is discretized into four types of particles: the wall particles, fluid particles, membrane particles and internal particles. The interaction between any two particles is characterized by the DPD approach. Apart from that, the membrane particles are subjected to the additional force generated by the cell deformation, which is described by the cell model. The motion of all the particles is governed by Newton's second law, and solved by the velocity-Verlet algorithm¹⁹. We first validate the DPD system by simulating the dynamic deformation of a spherical capsule in simple shear flow, and also check the effect of computational domain size on the capsule deformation. After that, we study the dynamic behaviors of a RBC in simple shear flow at different membrane shear and bending moduli, respectively.

2. Model Formulation

The simulation system is discretized into four types of particles: wall particles, fluid particles, membrane particles and internal particles, which move in accordance with Newton's second law,

$$m_i \frac{d^2 \mathbf{r}_i}{dt^2} = \sum_{j \neq i} \mathbf{f}_{ij}^{DPD}, \quad i \in P_f \cup P_i \quad (1)$$

$$m_i \frac{d^2 \mathbf{r}_i}{dt^2} = \sum_{j \neq i} \mathbf{f}_{ij}^{DPD} + \mathbf{f}_i^{DEF}, \quad i \in P_m \quad (2)$$

where m_i and $\mathbf{r}_i$ are the mass and position of the i^{th} particle; t is the time; P_f , P_i and P_m are the sets of fluid particles, internal particles and membrane particles; $\mathbf{f}_{ij}^{DPD}$ is the DPD force between the i^{th} and j^{th} particles; $\mathbf{f}_i^{DEF}$ is the membrane deformation force on the i^{th} particle including the elastic and viscous parts. Note that there is no equation governing the motion of wall particles, because the wall particles is set to be frozen for representing the system boundary.

2.1. DPD model

The DPD approach is used to model the external and internal fluids of a RBC, as well the interaction between the fluids and the RBC. It consists of three parts: a conservative part $\mathbf{f}_{ij}^C$, a dissipative part $\mathbf{f}_{ij}^D$ and a random part $\mathbf{f}_{ij}^R$,

$$\mathbf{f}_{ij}^{DPD} = \mathbf{f}_{ij}^C + \mathbf{f}_{ij}^D + \mathbf{f}_{ij}^R. \quad (3)$$

The conservative force is related to the compressibility of fluid, and the dissipative force mainly determines the viscosity of fluid. The random force makes a significant contribution to maintain a constant temperature in the system. They are defined as²⁰

$$\mathbf{f}_{ij}^C = \alpha_{ij} \omega^C(r_{ij}) \hat{\mathbf{r}}_{ij}, \quad (4)$$

$$\mathbf{f}_{ij}^D = -\gamma_{ij} \omega^D(r_{ij}) (\hat{\mathbf{r}}_{ij} \cdot \mathbf{v}_{ij}) \hat{\mathbf{r}}_{ij}, \quad (5)$$

$$\mathbf{f}_{ij}^R = \sigma_{ij} \omega^R(r_{ij}) \xi_{ij} / \sqrt{dt} \hat{\mathbf{r}}_{ij}, \quad (6)$$

where α_{ij} , γ_{ij} and σ_{ij} are the coefficients to characterize the force strengths; ξ_{ij} is a normally distributed random variable with zero mean and unit variance; dt is the time step; $\omega^C(r_{ij})$, $\omega^D(r_{ij})$ and $\omega^R(r_{ij})$ are weight functions; $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$, $r_{ij} = |\mathbf{r}_{ij}|$, $\hat{\mathbf{r}}_{ij} = \mathbf{r}_{ij} / r_{ij}$; and $\mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j$ in which $\mathbf{v}_i$ is the velocity of i^{th} particle. The conservative and dissipative weight functions are defined as

$$\omega^C(r_{ij}) = \begin{cases} (1 - r_{ij} / r_c), & r_{ij} < r_c, \\ 0, & r_{ij} \leq r_c, \end{cases} \quad (7)$$

$$\omega^D(r_{ij}) = \begin{cases} (1 - r_{ij}/r_c)^s, & r_{ij} < r_c, \\ 0, & r_{ij} \leq r_c, \end{cases} \quad (8)$$

where r_c is the cut-off radius; s is the exponent of dissipative force. The random weight function is determined by the fluctuation dissipation theorem²⁰ to maintain a constant temperature in the DPD system

$$\omega^R(r_{ij}) = \sqrt{\omega^D(r_{ij})}, \quad (9)$$

with the constraint

$$\sigma_{ij}^2 = 2k_B T \gamma_{ij}, \quad (10)$$

where $k_B T$ is the Boltzmann temperature.

2.2. Cell model

A whole RBC is discretized into membrane particles and internal particles, and the membrane particles are connected by non-linear worm-like chains²¹ with an additional viscous term into a viscoelastic triangular network. The membrane deformation force is thus expressed as

$$\mathbf{f}_i^{DEF} = \mathbf{f}_i^{ela} + \mathbf{f}_i^{vis}, \quad (11)$$

where $\mathbf{f}_i^{ela}$ and $\mathbf{f}_i^{vis}$ are the elastic and viscous parts, respectively.

The elastic part is determined by the total free energy U_{total} of the triangular network, defined as

$$\mathbf{f}_i^{ela} = \frac{\partial U_{total}}{\partial \mathbf{r}_i}. \quad (12)$$

The total energy includes the in-plane energy $U_{in-plane}$ describing the stretching deformation, the bending energy $U_{bending}$ describing the bending deformation, the area-constraint energy U_{area} describing the area conservation, and the volume-constraint energy U_{volume} describing the volume conservation⁶,

$$U_{total} = U_{in-plane} + U_{bending} + U_{area} + U_{volume}. \quad (13)$$

The in-plane energy is characterized by non-linear worm-like chains, given by

$$U_{in-plane} = \sum_{j=1}^{N_c} \left(\frac{k_B T l_j^{max}}{4 p_j} \frac{3x_j^2 - 2x_j^3}{1 - x_j} + \frac{k_j}{l_j} \right), \quad x_j = \frac{l_j}{l_j^{max}}, \quad (14)$$

where l_j and l_j^{max} are the current and maximum length of the j^{th} chain; N_c is the number of worm-like chains; $k_B T$ is the Boltzmann temperature; p_j is the persistence length; and k_j is a repulsive coefficient. The bending energy is described by the two adjacent triangles, defined as

$$U_{bending} = \sum_{j=1}^{N_c} k_b (1 - \cos(\theta_j - \theta_j^S)), \quad (15)$$

where k_b is the bending coefficient; θ_j is the instantaneous angle between two adjacent triangles having the common j^{th} edge; θ_j^S is the corresponding spontaneous angle. The area-constraint energy includes the local triangular and global network energies, given by

$$U_{area} = \frac{k_{glo} (A_{glo} - A_{glo}^{des})^2}{2A_{glo}^{des}} + \sum_{j=1}^{N_t} \frac{k_{loc} (A_j - A_j^{des})^2}{2A_j^{des}}, \quad (16)$$

where k_{glo} and k_{loc} are the global and local area-constraint constants; A_{glo} and A_j are the areas of the network and j^{th} triangle; A_{glo}^{des} and A_j^{des} are the corresponding desired areas; N_t is the number of triangles on the network. Similarly, the volume-constraint energy is defined as

$$U_{volume} = \frac{k_v (V - V^{des})^2}{2V^{des}}, \quad (17)$$

where k_v is the volume-constraint constant, V and V^{des} are the current and desired global volumes of the cell.

The viscous part should be related to the velocity as a damping role, which is modeled by the general fluid particle model²²

$$\mathbf{f}_i^{vis} = \sum_{j \in C_i} (\mathbf{f}_{ij}^{vis,D} + \mathbf{f}_{ij}^{vis,R}), \quad (18)$$

in which C_i is a set of the particle j connected into a chain with the particle i together; $\mathbf{f}_{ij}^{vis,D}$ and $\mathbf{f}_{ij}^{vis,R}$ are the dissipative and random parts defined by

$$\mathbf{f}_{ij}^{vis,D} = -\gamma^T \mathbf{v}_{ij} - \gamma^C (\mathbf{v}_{ij} \cdot \hat{\mathbf{r}}_{ij}) \hat{\mathbf{r}}_{ij}, \quad (19)$$

$$\mathbf{f}_{ij}^{vis,R} = \sqrt{2k_B T} \left(\sqrt{2\gamma^T} d\mathbf{W}_{ij}^S + \frac{\sqrt{3\gamma^C - \gamma^T}}{3} tr[d\mathbf{W}_{ij}] \mathbf{I} \right) \cdot \hat{\mathbf{r}}_{ij}, \quad (20)$$

where γ^T and γ^C are the dissipative parameters; $\mathbf{I}$ is the unit second-order tensor, $tr[d\mathbf{W}_{ij}]$ is the trace of a random matrix formed by independent Wiener increments $d\mathbf{W}_{ij}$; $\overline{d\mathbf{W}_{ij}^s}$ is the traceless symmetric part of $d\mathbf{W}_{ij}$. The random force part is included in Eq. (20) to keep a constant system temperature via a fluctuation-dissipation theorem.

Note that the cell model is not associated with the macroscopic properties. Fedosov *et al.*⁶ conducted a linear analysis for a regular hexagonal network, and expressed the macroscopic membrane shear modulus E_s , membrane bending modulus E_b , area dilation modulus E_d , and membrane viscosity μ_m as

$$E_s = \frac{\sqrt{3}k_B T}{4p_j l_{j,0}} \left[\frac{x_0}{2(1-x_0)^3} - \frac{1}{4(1-x_0)^2} + \frac{1}{4} \right] + \frac{3\sqrt{3}k_j}{4l_{j,0}^3}, \quad x_0 = \frac{l_{j,0}}{l_{j,0}^{max}}, \quad (21)$$

$$E_b = \frac{2}{\sqrt{3}} k_b, \quad (22)$$

$$E_d = 2E_s + k_{glo} + k_{loc}, \quad (23)$$

$$\mu_m = \sqrt{3}\gamma^T + \frac{\sqrt{3}\gamma^C}{4} \quad (24)$$

where the subscript ‘0’ refers to the stress-free state. Note that the membrane viscosity described by Eq. (24) is a partial membrane viscosity, which includes the contribution of DPD system in Eqs.(4)-(6).

2.3. Numerical method

The velocity-Verlet algorithm¹⁹ is adopted to solve Eqs. (1) and (2) to update the particle positions, and its scheme is given by

$$\mathbf{r}_i(t + \Delta t) = \mathbf{r}_i(t) + \Delta t \mathbf{v}_i(t) + 0.5 \Delta t^2 \mathbf{a}_i(t), \quad (25)$$

$$\tilde{\mathbf{v}}_i(t + \Delta t) = \mathbf{v}_i(t) + \lambda \Delta t \mathbf{a}_i(t), \quad (26)$$

$$\mathbf{a}_i(t + \Delta t) = \mathbf{F}_i(t + \Delta t) / m_i, \%(\mathbf{r}_i(t + \Delta t), \tilde{\mathbf{v}}_i(t + \Delta t)), \quad (27)$$

$$\mathbf{v}_i(t + \Delta t) = \mathbf{v}_i(t) + 0.5 [\mathbf{a}_i(t) + \mathbf{a}_i(t + \Delta t)], \quad (28)$$

where

$$\mathbf{F}_i(t + \Delta t) = \begin{cases} \sum_{j \neq i} \mathbf{f}_{ij}^{DPD}, & i \in P_f \cup P_i, \\ \sum_{j \neq i} \mathbf{f}_{ij}^{DPD} + \mathbf{f}_i^{DEF}, & i \in P_m. \end{cases} \quad (29)$$

In the above procedure, it is an important step to calculate the DPD force $\mathbf{f}_{ij}^{DPD}$ and the membrane deformation force $\mathbf{f}_i^{DEF}$. At the initial state, the locations of all the particles are given, and their velocities and accelerations are set to be zero. Therefore, the DPD force $\mathbf{f}_{ij}^{DPD}$ and the viscous part $\mathbf{f}_i^{vis}$ of the membrane deformation force are easily calculated by Eqs. (4)-(6) and Eqs. (19) and (20). For calculating the elastic part $\mathbf{f}_i^{ela}$ of the membrane deformation force, we treat the initial state of cell as the stress-free state, such that several parameters are calculated, including the persistent length p_j , the repulsive coefficient k_j , the spontaneous angle θ_j^S , the global desired area A_{glo}^{des} , the local desired area A_j^{des} , and the desired volume V_{des} . After that, the elastic part of membrane deformation is obtained, once we set the membrane moduli (shear modulus, bending modulus and area dilation modulus).

3. Results and Discussions

In this section, we first validate the DPD system coupled with the discrete cell model by simulating the dynamic behaviors of a spherical capsule in simple shear flow, and examine the effect of computational domain size. After that, we study the dynamics of a RBC in simple shear flow at different membrane shear and bending moduli, respectively.

3.1. Validation

To validate the present DPD system, we simulate the transient deformation of a spherical capsule in simple shear flow, and compare our results with Sui *et al.*'s¹². In our work, we set the membrane shear modulus $E_s = 6\mu N/m$, the bending modulus $E_b = 2.4 \times 10^{-19} J$, the shear rate $\dot{\gamma} = 1.96 \times 10^3 s^{-1}$, the fluid viscosity $\mu_o = 6.13 \times 10^{-4} pa \cdot s$, and the sphere radius $R = 3.0\mu m$. Hence, the capillary number is $Ca = \mu_o \dot{\gamma} R / E_s = 0.6$, which is used in Sui *et al.*'s work¹². Fig. 2 shows the evolution of Taylor deformation parameter (TDP) of a spherical capsule in the different computational domain sizes, and the TDP is defined as $D_{xz} = (L - W) / (L + W)$ where L and W are the major and minor radii of the capsule in the plane of shear. It can be found that our results are very close to the Sui *et al.*'s¹² before $\dot{\gamma}t = 2$. However, they are smaller than their results¹² after $\dot{\gamma}t = 2$, which is possibly ascribed to the random force in DPD system. The random force cannot keep the capsule center stationary, such that the capsule deformation slightly decreases with increasing time. Furthermore, the decreasing trend is more obvious in the computational domain of $15 \times 15 \times 15\mu m^3$, but similar in the rest three computational domains. Therefore, we take the computational domain of $20 \times 20 \times 20\mu m^3$ in the following simulations for saving the computational costs. Fig. 3 shows the cross-section of deformed capsule in simple shear flow, where the initial spherical capsule is stretched and tilts gradually to a steady shape with a stationary shape and fixed orientation.

Fig. 2. Temporal evolution of Taylor deformation parameter of a spherical capsule in the different computational domain sizes, compared with Sui *et al.*'s work¹².

Fig. 3. Cross-section of deformed capsule in simple shear flow at $\dot{\gamma}t = 0, 1, 2, 3, 4$, where the circular points show the membrane rotation.

3.2. Effect of membrane shear modulus

Fig. 4 illustrates the dynamic behaviors of RBCs with different shear moduli $E_s = 6, 60$ and $600 \mu N / m$ in simple shear flow, where the bending modulus is $E_b = 2.4 \times 10^{-19} J$. At $E_s = 6 \mu N / m$, the RBC tilts and is stretched, and finally approaches to a steady state with the a stationary shape and fixed orientation. This is well known as tank-treading motion. At $E_s = 600 \mu N / m$, the RBC tumbles continuously with negligibly small shape change, which is an unsteady state called the tumbling motion. In this case, the RBC is difficult to deform and flips subject to the shear flow due to the significant strong shear modulus. At $E_s = 60 \mu N / m$, the RBC is in a transitional state with both the tank-treading and tumbling motions. It has a periodic shape deformation and oscillatory orientation, and the membrane inward folding appears repeatedly, like the RBC breathing. This is the trembling motion, and also called the breathing motion.

Fig. 4. Dynamics of RBCs with different shear moduli in the simple shear flow, (a) tank-treading motion at $E_s = 6 \mu\text{N/m}$, (b) trembling motion at $E_s = 60 \mu\text{N/m}$, and (c) tumbling motion at $E_s = 600 \mu\text{N/m}$. The snapshots are taken at $\dot{\gamma}t = 0, 0.86, 1.72, 2.58, 3.44, 4.3, 5.16, 6.02$ and 6.88 from the left column to right column.

Fig. 5. Variations of (a) membrane area and (b) volume of RBCs with different shear moduli in the simple shear flow.

In Fig. 4, the RBC's area and volume seem not to be conserved, especially in the tank-treading and trembling motions. In fact, they are well conserved in our work, as illustrated in Fig. 5. With increasing the membrane shear modulus, the variation of RBC's area becomes smaller and smaller, and it almost has no change at $E_s = 600 \mu\text{N/m}$. Even at $E_s = 6 \mu\text{N/m}$, it increases by a maximum of 1%. This is attributed to the strong area constraint used in our work, for describing the fact that the real RBC can strongly conserve the surface area. Moreover, the RBC's volume is also almost conserved with the maximum volume variation of 0.1%, because the RBC is assumed to be impermeable. It is found in Fig. 5 that the RBC's area and volume exhibit a periodic characteristics, especially the RBC's area at $E_s = 6 \mu\text{N/m}$. This is because the RBC has a slight and periodic shape variation. In turn, the slight and periodic shape variation mainly results from the random force in DPD system, leading to the RBC's center moving.

3.3. Effect of membrane bending modulus

Fig. 6 shows the dynamic behaviors of RBCs with different bending moduli $E_b = 2.4 \times 10^{-19}$, 2.4×10^{-18} and 2.4×10^{-17} J in simple shear flow, where the shear modulus is $E_s = 6$ μ N/m. At $E_b = 2.4 \times 10^{-19}$ J, the RBC undergoes a tank-treading motion. However, it undergoes a trembling motion at both $E_b = 2.4 \times 10^{-18}$ and 2.4×10^{-17} J, and the shape deformation is almost identical in these two cases. At the low bending modulus, the RBC is stretched to have two relatively sharp end-parts subject to the shear flow, and further developed to be a streamlined shape. As a result, the tank-treading motion occurs. At the high bending modulus, however, the RBC has strong resistance to the bending deformation, especially at the part with large curvature, such that the sharp end-parts are smoothed and the streamlined shape cannot be reserved any more. Therefore, the RBC's stretching and smoothing coexist in this case and occur alternately. Meanwhile, there is a critical value of bending modulus. If the bending modulus is larger than the critical value, the bending modulus has no effect on the dynamic behaviors of RBC. That's why the RBC deformation is almost identical at both $E_b = 2.4 \times 10^{-18}$ and 2.4×10^{-17} J.

Fig. 6. Dynamics of RBCs with different bending moduli in the simple shear flow, (a) tank-treading motion at $E_b = 2.4 \times 10^{-19}$ J, (b) trembling motion at $E_b = 2.4 \times 10^{-18}$ J, and (c) trembling motion at $E_b = 2.4 \times 10^{-17}$ J. The snapshots are taken at $\dot{\gamma}t = 0, 0.86, 1.72, 2.58, 3.44, 4.3, 5.16, 6.02$ and 6.88 from the left column to right column.

4. Conclusions

We have presented a DPD system coupled with a discrete cell model to numerically investigate the dynamics of a RBC in simple shear flow. The simulation system is discretized into the four types of particles, namely the wall particles, fluid particles, membrane particles and internal particles. The interaction between any two particles is characterized by the DPD approach, and the membrane particles are connected into a network subject to the membrane deformation force. The membrane deformation force is described by the discrete cell model, including the in-plane force resulted from the stretching deformation, the bending force from the bending deformation, the area-constraint force from the area change, and the volume-constraint force from the volume change. The motion of all the particles is governed by Newton's second law, and solved by the velocity-Verlet algorithm. We validate the DPD system by simulating the dynamic

deformation of a spherical capsule in simple shear flow, and further examine the effect of computational domain size on the capsule deformation. After that, we study the dynamic behaviors of a RBC in simple shear flow at different membrane shear and bending moduli, respectively. Our simulations reproduce the tank-treading, trembling and tumbling motions of RBCs at the shear modulus $E_s = 6, 60$ and $600 \mu\text{N/m}$, respectively. In addition, we find that the RBC undergoes a trembling motion when its bending modulus is large enough, in which the RBC's stretching from the shear flow and the RBC's smoothing from the large bending modulus occur alternately in shape.

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