Simulating Transport of Soft Matter in Micro/Nano Channel Flows with Dissipative Particle Dynamics

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The flow-induced transport of various soft matter systems through a fluidic channel has recently attracted great interest due to its significance ranging from the understanding of several chemical and biological processes to potential industrial and technical applications. Dynamic simulation and modeling can yield an insight into the detailed conformational, dynamical, and transport properties of soft matter systems, which is necessary to understand the transport properties of biological macromolecules in living organisms. As a mesoscopic particles-based simulation technique, dissipative particle dynamics (DPD) has quickly been adopted as a promising approach for simulating dynamic and rheological properties of simple and complex fluids as well as the events taking place inside the fluidic channels. Here, the DPD method widely used in predicting the channel flow containing various soft matter systems is reviewed. The general aspect and basic formulations of DPD are introduced, and different boundary conditions are presented for wall-bounded flows. In addition, the models based on DPD developed to simulate flow-induced transport through fluidic channels for some typical soft matter systems are discussed, including red blood cells, vesicles, polymers, and biomacromolecules. Finally, the future directions to signify the framework in enhancing the design of novel functional systems and beyond are discussed.

1. Introduction

The transport of soft matter systems through a micro- and nanofluidic channel is of great significance in the understanding of some biological and chemical processes such as the motion of DNA and RNA across narrow pores, translocation of proteins through the channels of cell membrane, and infection of virus into the cell nucleus.[1–3] Such a dynamical process can also lead to several potential technical and industrial applications including genomic partitioning techniques, rapid DNA sequencing, and transport cargo for drug delivery into biological cells.[4–6] It is not surprising that the transport of soft matter has become a subject of intensive experimental,[6–9] theoretical,[10–13] and computational studies[14–20] as it bears many interesting applications and is essential in the understanding of many fundamental processes in materials, physics, and biology sciences.

Extensive experimental studies have been conducted to investigate the transport processes of various soft matter systems through a fluidic channel. For example, Wu and co-workers[21] observed that polymer chains can pass through narrow pores much smaller than their unperturbed radius via a special double-layer membrane to avoid interaction among flowfields, confirming the prediction of Sakaue et al.[22] that the critical suction current in linear polymers is independent of the degree of polymerization. The microcirculatory network of blood vessels in the body primarily serves as the conduit for the exchange of gases between blood and tissues, through the red blood cells (RBCs).[23] Experimental studies showed that RBCs often arrange themselves into a single file, when passing through a narrow tube with a diameter comparable to a RBC diameter (about 10 µm).[24] or a slightly wide tube with a diameter of about 25 µm but at a high fluid viscosity.[25] In fact, the motion of deformable particles in a flow is the subject of intensive studies in various contexts. Several experimental studies have also been performed on microchannel or confined flows of vesicles because vesicles differ from other deformable objects due to a nearly constant volume on experimental time, a low bending modulus, and the fluid state of their membrane in contrast to the elastic solid state of the membrane of a capsule.[26–30] The dynamic and rheological properties of single-strand DNA molecules in a channel flow have also been extensively studied.[31] For instance, fluorescence imaging techniques have been used to visualize the microstructural conformations of molecules in flows.[32]

Despite these experimental studies, many important aspects of hydrodynamic flow field as a transport mechanism remain unexplored, requiring a more fundamental study on the transport of soft matter systems through fluidic channels. Such studies may deepen understanding of the detailed structural changes of soft matter inside the fluidic channels. When an experiment encounters difficulties, tailored computer simulations offer alternative approaches, with their unique ability to identify and separate...
individual contributions to the phenomena or processes of interest. Indeed, dynamical simulation and modeling have demonstrated their advancement in predicting how various soft matter systems behave in fluidic flows and channels.\textsuperscript{33–38} Particularly, particle-based methods, such as molecular dynamics (MD), dissipative particle dynamics (DPD), and smoothed particle hydrodynamics (SPH), have been increasingly attractive for solving fluidic flow problems because of the ease and flexibility in modeling complex structure fluids afforded by the methods.

This review thereby focuses on one of the most popular particle-based methods widely used in dealing with the issues regarding the transport of soft matter systems through fluidic channels, that is, DPD.\textsuperscript{39,40} This method is originally designed as a mesoscopic particle-based simulation technique by Hoogerbrugge and Koelman,\textsuperscript{39} and is quickly adopted as a promising approach for simulating dynamic and rheological properties of simple and complex fluids, such as multiphase fluids and cell suspensions (Figure 1). The general aspect and basic formulations of DPD, boundary conditions for wall-bounded flows, as well as some typical soft matter systems are introduced regarding the applications of DPD in simulating flow-induced transport through fluidic channels. We hope that this review will shed light on the understanding of the transport properties of various soft matter systems and the development of skills for the current and future fluidic technologies.

2. Method and Boundary Conditions

2.1. General Aspect of Dissipative Particle Dynamics

In this review, the research results we introduced are mainly simulated by DPD, which was first proposed by Hoogerbrugge and Koelman in 1992.\textsuperscript{39,40} After that, Espa˜nol and Warren\textsuperscript{41} successfully combined the dissipative-fluctuation theorem with the DPD method, laying a solid foundation for statistical mechanics. Taking into account the limitation in the time and length scales in simulation, the DPD simulation method bridges the gap between atomistic and mesoscopic simulation, which has been broadly used in many areas.\textsuperscript{42–45} In DPD method, each bead represents a cluster of atoms, and the position of the bead is the mass center of the cluster. The interaction forces between the beads $i$ and $j$ include three types, conservative force $\mathbf{F}_C^i$, dissipative force $\mathbf{F}_D^i$, and random force $\mathbf{F}_R^i$, that is, $\mathbf{f}_i = \sum_{j \neq i} \left( \mathbf{F}_C^i + \mathbf{F}_D^i + \mathbf{F}_R^i \right)$. The interaction forces are paired and acting within a certain cutoff radius $r_c$. The conservative force is a soft repulsion and is given by

\begin{equation}
\mathbf{F}_C^i = \begin{cases} a_{ij} \left( 1 - r_{ij} \right) \mathbf{r}_{ij} & \left( r_{ij} > 1 \right) \\ 0 & \left( r_{ij} \geq 1 \right) \end{cases}
\end{equation}

where $a_{ij}$ is the maximum repulsion between beads $i$ and $j$, and $r_{ij} = r_i - r_j$, $r_{ij} = |r_{ij}|$, $\mathbf{r}_{ij} = r_{ij}/|r_{ij}|$. The larger the value of $a_{ij}$, the greater the repulsive force between beads $i$ and $j$, where $a_{ii} = 25$ is the repulsion parameter between like species. The dissipative force and the random force are given by

\begin{equation}
\mathbf{F}_D^i = -\gamma \omega D \left( r_{ij} \right) \left( \mathbf{r}_{ij} \cdot \mathbf{v}_{ij} \right) \mathbf{r}_{ij}, \quad \mathbf{F}_R^i = \sigma \omega R \left( r_{ij} \right) \zeta_{ij} \Delta t^{-1/2} \mathbf{r}_{ij}
\end{equation}

where $\mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j$; $\omega D$ and $\omega R$ are weight functions and conform to the formula $\omega D \left( r_{ij} \right) = [\omega^D \left( r_{ij} \right)]^2 = \left( 1 - r_{ij} \right)^2$ for $r_{ij} < 1$; $\zeta_{ij}$ is a random number with zero mean and unit variance; $\Delta t$ is the time step in simulation; $\gamma$ is a simulation parameter related to viscosity and $\sigma^2 = 2\gamma k_B T / k_B$ and $T$, respectively, represent Boltzmann constant and the temperature. All simulations are based on a modified version of the velocity-Verlet algorithm as follows.

\begin{equation}
\mathbf{v}_i \left( t + \Delta t \right) = \mathbf{v}_i \left( t \right) + \Delta t \mathbf{v}_i \left( t \right) + \frac{1}{2} \left( \Delta t \right)^2 \mathbf{F}_i \left( t \right),
\end{equation}

\begin{equation}
\mathbf{v}_i \left( t + \Delta t \right) = \mathbf{v}_i \left( t \right) + \lambda \Delta t \mathbf{F}_i \left( t \right)
\end{equation}
Figure 1. Schematic diagram of the applications of DPD in the simulations of flow-induced transport of various soft matter systems: (top left) vesicles, (top right) red blood cells, (bottom left) polymers, and (bottom right) biomacromolecules.

\[ f_i(t + \Delta t) = f_i \left( \mathbf{r}(t + \Delta t), \mathbf{v}(t + \Delta t) \right) \]

\[ v_i(t + \Delta t) = v_i(t) + \frac{1}{2} \Delta t \left( f_i(t) + f_i(t + \Delta t) \right) \]

2.2. Lees–Edwards Boundary Condition

The fluids are simulated by a collection of DPD beads, and in order to obtain the hydrodynamic flow field, the most common method is to apply an external body force \( f_e \) parallel to the flow direction for each solvent bead in the channel. We usually choose to apply the force that gradually changes over time and finally tends to be constant, which can better prevent the transported objects from breaking or deforming due to the sudden application of external body force. By varying the body force, we can control the size of the applied flow field.

Boundary conditions have always been the focus of researchers in DPD simulations of wall-bounded flows. Especially for the complex geometry flows, a correct application of boundary conditions can make the results much more accurate. Because of the soft repulsion between DPD particles, we cannot prevent fluid beads from penetrating solid boundaries, and thus extra effort is required to impose accurately the no-slip wall boundary condition. Until now, there are three main approaches to impose boundary conditions in DPD simulation (Figure 2).

The Lees–Edwards boundary condition was first proposed to simulate shear flows by Lees and Edwards in 1972,[46] which is an effective way to avoid modeling the physical boundary (Figure 2A).[47] The middle rectangle in Figure 2A represents the computation domain, and the periodic boundary condition is set at the upper and lower boundaries. Once a particle \( i \) moves out of the computation domain, it will re-enter into the domain as particle \( i' \) from the opposite site. The velocity \( v \) and position \( x \) of the particle \( i \) need to be modified as follows:[48]

\[ x_i' = \begin{cases} \mod \left( (x_i - \gamma L_y t) \cdot L_x, L_x \right) , & y_i \geq \frac{L_y}{2} \\ \mod \left( (x_i + \gamma L_y t) \cdot L_x, L_x \right) , & y_i < -\frac{L_y}{2} \end{cases} \]

\[ y_i' = \mod \left( y_i, L_y \right) \]

(4)
where \( \text{mod} \) represents the modular function; \( L_x \) and \( L_y \) are the length and width of the computation domain, respectively; and \( \dot{\gamma} \) is the imposed shear rate parallel to the \( x \)-axis direction. So, the periodic domains are shifted with a velocity \( \dot{y} L_y / 2 \).

With the Lees–Edwards boundary method,\[49–51\] the velocity and distribution of the particles at the upper and lower boundaries will not have a severe fluctuation, which is a great advantage. However, the Lees–Edwards boundary method is mainly applied to some simple shear flows, such as Couette flow. As it is difficult to be applied to handle more complex flows, this method has not been widely used by researchers.

2.3. Solid Wall with Freezing DPD Beads

The second method is to simulate the solid wall by freezing some DPD beads.\[52–54\] The frozen beads are fixed at certain positions on the wall where they can interact with other beads, but are not allowed to move (Figure 2B). In order to prevent the solvent beads from penetrating the wall, researchers choose to increase the wall density as well as the repulsive force between wall beads and solvent beads. However, this solution will cause large fluctuations in flow velocity and bead density near the wall regions. According to the simulation results of Pivkin et al.,\[55\] we can conclude that increasing the wall bead density or the repulsive force may not be a very effective solution.

2.4. Bead-Layers with Proper Reflections

The third method has some modifications based on the second one,\[56,57\] as it combines different types of bead-layers with proper reflections, mainly including bounce forward reflection, bounce back reflection, specular reflection, and Maxwellian reflection (Figure 2C).\[58\] Once a solvent bead penetrates the wall, the reflection can reflect the bead back into the fluid. In specular reflections, the velocity component parallel to the wall is conserved and the normal component is reversed, while in the bounce forward/back reflection both velocity components are reversed. In the Maxwellian reflection, the beads are returned into the fluid with a velocity following a Maxwellian distribution.\[59\] This method can be further implemented by setting an extra thin layer of DPD beads adjacent to the solid wall, which has a thickness of 0.5% of the height of the channel. This extra thin layer can be thought of as a “buffer”. When a DPD bead enters into this layer, a new velocity is obtained from the formula

\[
v_i = v_R + n(\sqrt{(n \cdot v_R)^2 - n \cdot v_S})
\]

where \( v_R \) is the random velocity generated by the Maxwell distribution and \( n \) is the unit vector toward the flow region. Then the bead will re-enter into the flow field with velocity \( v_i \). This third category of boundary condition

\[
\begin{align*}
&v_{x_f} = \begin{cases} 
  v_x - \dot{y} L_y, & y_i \geq L_y / 2 \\
  v_x + \dot{y} L_y, & y_i < -L_y / 2
\end{cases} \\
v_{y_f} = v_y
\end{align*}
\]

Figure 2. Schematic diagram of several boundary conditions. A) Lees–Edwards boundary condition. Reproduced with permission.\[47\] Copyright 2018, The American Institute of Physics. B) Freeze some particles to create a rigid wall. Reproduced with permission.\[52,55\] Copyright 2005, Elsevier; Copyright 1994, The Springer Nature. C) Employ collections of frozen particles in combination with proper reflections. (a) Bounce forward/back reflection. (b) Specular reflection. Reproduced with permission.\[58\] Copyright 2012, Elsevier.
methods has been widely applied to the simulation of various complex fluids through some different designs and changes.\[60-62\]

3. Transport of Some Soft Matter Systems

3.1. Red Blood Cells

RBCs are the most abundant blood cells in the blood, accounting for about 40% of the volume concentration. They are the most important medium for transporting oxygen through the blood in the human body and also have certain immune functions. Because of the essential role in blood circulation, as early as the 1970s,\[63\] many researchers began to explore the flow of blood and the shape evolution of RBCs as they flow in the blood vessels.

Among them, the morphological changes of RBCs are of major concern to the scientists because it is closely related to the physiological functions of RBCs. Blood vessels of the human body can be divided into various types such as aorta, arteriole, vena cava, veinlet, and capillary, in which the diameters, flow rates, surface roughness, and other conditions are distinctly different. These factors can cause obvious morphological changes of RBCs during the transport process. Computer simulation can help us better observe the process of RBC shape evolution\[33,64,65\] and provide reliable theoretical analysis for experimental research (Figure 3).

In general, two classic models can be used to simulate RBCs in the DP simulation, which are the low-dimensional model and the spectrin-level model.\[60\] The low-dimensional RBC model is based on a ring of \(N_c\) colloidal particles connected by wormlike chain (WLC) springs, and each colloidal particle is represented by a single DPD bead with a new DPD formulation.\[67\] The WLC spring force is given by

\[
F_{\text{WLC}} = k_p \left[ \frac{1}{4(1 - \frac{r_{ij}}{L_{\text{max}}})^2} - 1 + \frac{r_{ij}}{L_{\text{max}}} \right]
\]

where \(k_p\) is the persistence length and \(L_{\text{max}}\) is the maximum spring extension. Although increasing the beads number \(N_c\) can result in better agreement, it will increase the calculation cost. Therefore, under the guarantee of sufficient agreement, researchers generally choose \(N_c = 10\). The spectrin-level model consists of \(N_c\) DPD beads, which are vertices of a 2D triangulated network on the RBC surface.\[68\] The length of the link between beads \(m\) and \(n\) is given by \(L_{ij} = |x_m - x_n|\). The free energy of the system is given by

\[
V([x_i]) = V_{\text{in-plane}} + V_{\text{bending}} + V_{\text{area}} + V_{\text{volume}}
\]

The detailed calculation formulas can be found in ref. \[65\]. To obtain an initial biconcave RBC shape, the coordinates of the vertices satisfy the following equation.

\[
y = R \sqrt{1 - \frac{x^2 + z^2}{R^2}} \left[ c_0 + c_1 \frac{x^2 + z^2}{R^2} + c_2 \left( \frac{x^2 + z^2}{R^2} \right)^2 \right]
\]

where the parameter \((R, c_0, c_1, c_2) = (3.91 \, \mu m, 0.1035805, 1.001279, -0.561381)\).\[65\] The larger the beads number \(N\), the smoother the surface of the RBC model appears. The evolution of the coordinates and the velocity of the \(N\) DPD beads modeled RBC are governed by Newton’s equations of motion.

\[
\frac{dx_i}{dt} = v_i; \quad \frac{dv_i}{dt} = f_i + f_{\text{ext}}^i
\]

where the force \(f_i = -\frac{\partial V}{\partial x_i}\), \(v_i\) is velocity, and \(f_{\text{ext}}^i\) is the externally applied force on the bead. In order to ensure that the model can accurately represent RBC, \(N\) is preferably greater than 250. In general, the spectrin-level model is more widely used because it is closer to the actual shape of RBC, which can accurately capture the 3D geometry and viscoelasticity.

Pivkin and Karniadakis\[69\] investigated the deformation of a RBC flowing in a microchannel, as indicated by the schematic diagram in Figure 3A(a–c). The simulated cylindrical channel has a diameter of 10 \(\mu m\), which is slightly larger than the diameter of a human RBC, 8 \(\mu m\). Initially, the RBC is in the center of the flow channel with a bicone shape. With the application of the driving force, the RBC begins to move in the channel, and the deformation into a parachute shape can be observed. Furthermore, after removing the driving force, the flow slows down and eventually returns to rest while the RBC simultaneously recovers its initial bicone shape. This fully reflects the high deformability and shape memory characteristics of RBCs. The high deformability ensures that RBCs will not rupture when transiting through narrow blood vessels.\[70,71\] From the experiment we can also observe the deformation (Figure 3A(e)).\[72\]

Ye’s group demonstrated the shape evolution of a RBC in different types of channels, including rectangular, straight cylindrical, curved cylindrical, and bifurcate tubes (Figure 3B).\[73\] When flowing in the rectangular and the straight cylindrical tubes, the RBC rapidly changes from a biconcave to parachute shape under the action of the flow field. Due to the symmetry of the flow channels, the shapes of the deformed RBCs are also highly symmetrical. However, in the curved cylindrical and bifurcate tubes, the asphericity of the RBCs fluctuates with the flow path. In particular, when flowing in the narrow bifurcated flow path, the RBCs change from a parachute shape to a slipper shape, and are more likely to be close to the wall. Such deformation is more conducive to the transportation of RBCs in the flow channel smaller than their own diameter, because it ensures that the flow rate is not too slow and prevents clogging of RBCs as they flow through the channel.

Through the combination of experiment and simulation, Guckenberger et al.\[74,75\] reported that the flow velocity is also a major factor determining the morphology of RBCs. From Figure 3C(a), we can observe that in a certain diameter of the flow channel, as the flow velocity increases, RBCs gradually change from the equilibrium biconcave shape, the croissant shape, to the slipper shape. In general, the larger the velocity, the more slender and flattened the shape of RBCs. Figure 3C(b, c) show the morphologies of the RBCs at the velocity of 1.1 \(mm \cdot s^{-1}\) and 5.2 \(mm \cdot s^{-1}\), are respectively the typical croissant and slipper shapes, which exactly matches the experimental results observed at the same velocity in Figure 3C(a). The findings of Bento et al.\[76\]
also fully illustrated the important effects of flow channel width and velocity on RBC deformability (Figure 3D).

Fedosov found that RBCs, freely dispersed in the blood, will be concentrated at the center of the flow channel after passing through a constriction, indicating that the constriction has the function of enriching the distribution of RBCs. They also found that when particles and RBCs are presented in the flow channel, the distribution of particles in the channel is not only related to the velocity and the width of the channel. The hematocrit value ($H_v$), which is defined as the volume fraction of RBCs, is also an important factor (Figure 3E). The particle surfaces are colored according to their radial position in the channel, with yellow color indicating a position near the center, while blue color corresponds to a position near the wall. The simulation results show that in the case of large $H_v$, the particles tend to be distributed and moved away from the center of the flow channel. In other words, as $H_v$ increases, the particles show a better margination property.

This provides a very useful reference for the application of particles as drug-delivery carriers for transport under realistic blood flow environment.

In addition, numerous studies have also shown that RBCs undergo more severe deformation at the same velocity as they move in a channel coated with polymer brushes compared to that in a bare channel. At the same time, the presence of the brushes will reduce the flow velocity and affect the flow pattern. This is more in line with the actual situation, because there are proteins adhering on the blood vessel wall of the human body.

3.2. Vesicles

Amphiphilic molecules can form vesicles by self-assembly. Vesicles are one of the important 3D self-assemblies, and their unique hollow structure makes them widely used in many fields.
such as drug transport, temporary storage of food and enzymes, and chemical reaction chambers. The vesicles in the simulation systems are usually self-assembled from amphiphilic molecules. Each amphiphilic molecule is composed of several DPD beads, which contain a hydrophilic head and a hydrophobic tail. The spring force between adjacent beads can be calculated through the formula $F = K_{\text{bond}} \frac{(r_{ij} - b)}{r_c}$, where $K_{\text{bond}}$ is the bond constant and $b$ is the equilibrium bond length.

As mentioned already for the work of Chu and co-workers, the behavior of multicomponent vesicles under Poiseuille flow in a channel is related to the Reynolds number ($Re$) and the concentration of the key component (Figure 4A). The shape of the vesicles changes from an initial symmetric sphere to an asymmetric bullet-like shape with the increasing of Re. In the case of high concentrations of hairy lipids, the overall deformation trend of the vesicles is similar, but we can observe that the degree of deformation is smaller than that with the low concentration. Such simulation results indicate that the presence of hairy lipids enhances the ability of vesicles to resist deformation. When $Re$ exceeds a critical value, the vesicles cannot withstand the flow field force, excessive deformation occurs, and they finally rupture (Figure 4D). The mechanism of rupture can be roughly divided into several stages. First, due to the turbulence caused by the strong flow, some molecules are pushed from the bilayer and form a tail (Figure 4D(a)). Then, with the constant loss of molecules, the surface of the vesicles begins to create a pore, and it continues to increase under the action of the flow field force. Eventually, vesicles rupture completely.
Ye and Coupier et al. investigated through simulations and experiments that vesicles tend to be crescent or parachute shapes in narrower flow channels, while prefer tapered or bullet-like shape in wide channels (Figure 4B(a–c)). Therefore, by controlling the flow channel width and velocity, Yamada et al. designed a device for trapping or releasing the giant unilamellar vesicles (GUVs) in a microfluidic channel. The results indicated that GUVs whose diameters are slightly larger than the channel height can be trapped in the well and that they can be released by flowing the outer fluid beyond a critical velocity (Figure 4B(d)).

When translated through a narrow constriction in the channel, the shape change of the vesicle usually goes through three stages, as indicated by the schematic diagram in Figure 4C for the work of Bertrand and Kusters et al.: Stage I, free suspension in the flow channel with a sphere shape; Stage II, partial entry of the vesicle into the narrow constriction; Stage III, vesicle flow in the constriction with a shape of spherocylindrical. However, in Stage II and Stage III, the vesicles may be broken due to the extrusion or stuck in the narrow constriction. Phase diagrams in Figure 4C(d) discussed several factors that influence whether a vesicle can pass through the constriction successfully, including the relative size of the constriction $d/R_0$, the constriction length $L$, and the driving force $F_m$.

Balazs et al. simulated vesicle as a carrier for transporting matter. In their simulation work, the vesicle is able to pick up several Janus particles in the flow channel and drop off them when it reaches a particular location (Figure 4E(a)). The size and polydispersity of the vesicle, the interaction between vesicle, Janus particles and channel wall, and the flow velocity all influence the effect of the vesicle deliver process.

Barakat and Shaqfeh developed a rigorous theory for the motion of a vesicle flowing through a narrow tube, and the theoretical predictions were in great agreement with the experimental results. Aranda et al. simulated the transport of a vesicle within a peristaltic tube. Therefore, in practical applications, these conclusions from the simulation works by Aranda and Barakat can be combined to design the vesicles, so that vesicles can be better used to deliver drugs in different channel types in the human body. When vesicles reach the specific sites, they can recognize the receptors such as proteins and release the drugs accurately.

### 3.3. Polymers and Biomacromolecules

The translocation of polymers through a narrow channel or a narrow pore is a complicated but ubiquitous physical process. A series of chemical and biological processes, including DNA and RNA translocation across nuclear pores, protein transport through the channels on the cell membrane, etc., are closely related to it. DPD simulations can help us observe the traversal processes at mesoscopic scales, so that we can explicitly understand and elucidate the fundamental processes of biology and polymer sciences.

In general, the transport process of polymers in the flow channel is affected by some intrinsic or external factors, such as polymer length, channel types, solvent conditions, polymer morphology, type and magnitude of driving force. In recent years, a multitude of scientists have conducted research on the above-mentioned influencing factors and obtained some valuable results. These external and intrinsic factors determine whether the polymer can successfully pass through the channel and how long it takes to pass through the channel (Figure 5A(a)).

The translocation time $\tau$ is generally defined as the time internal between the first particle of the polymer chain entering the flow channel and the last particle passing through the channel. The first influencing factor considered is the chain length of polymer. In DPD simulations, we typically model the real polymer molecules as a chain of DPD beads. The chain length of the polymer chain in the simulation can be controlled by increasing or decreasing the beads. When the width of the flow channel is constant, as the length of the polymer chain increases, the probability of the failed translocation becomes greater. Guo et al. found that when the chain length exceeds a critical value, the polymer has a high probability of clogging at the entrance of the flow channel. Even if it successfully enters the channel, it is easily “fixed” during the transportation, because the oversized polymer size makes it difficult to make further conformation adjustment in the narrow channel, and the driving force is not powerful enough to push it forward. They also summarized a scaling relation with $\tau \sim N^{1/3}$ between the average translocation time $\tau$ and the polymer chain length $N$ in long chain length (Figure 5A, b), while $\tau$ is almost independent of $N$ in short chain length.

Solvent condition is another factor that is of concern to the researchers. Polymer chains usually exhibit a random coil state in the solvent, and the extension states of the chains change as the solvent conditions change. We can control different solvent qualities by changing the polymer–solvent interaction parameter $\alpha_{PS}$ in the simulation. The larger the value of $\alpha_{PS}$, the greater the repulsive force between the polymer and the solvent. When the quality of the solvent is changed from good to poor, different interaction forces between polymer beads and solvent beads will cause the polymer configuration transition from a swollen to a compact state (Figure 5B(b)). Yang et al. obtained the dependence of polymer translocation time $\tau$ on the solvent quality, which is shown in Figure 5B(c). From the comparison of the two graphs, they concluded that polymers translocate faster through the narrow pore under good solvent condition. Meanwhile, we can also find that the solvent quality has a greater impact on longer chains than shorter chains, indicating that changes in chain length are more sensitive under good solvent conditions.

Guo and co-workers demonstrated that the channel width and the value of driving force can affect the polymer chain conformation during the transport process. Even in the case where the equilibrated radius of gyration of a polymer chain is greater than the radius of the narrow channel, polymer chain can still successfully pass through the fluidic channel through adjustment of the conformation. For linear polymer chains, they can pass through the channel in single-file or multi-folded (double or triple) conformations (Figure 5C(b)). Basically, the translocation process of linear polymers can be divided into three stages as indicated by the schematic diagram in Figure 5C(a): 1) drift diffusion, 2) capture, and 3) translocation. During translocation through the narrow channel, the polymer chain is stretched and the mean square radius of gyration will increase dramatically, which is a process of entropy increase. As the driving force increases,
polymer chains tend to translocate within a multi-folded conformation. Such a conformational transition is also ubiquitous when many biomacromolecules cross the narrow channel. For example, the majority of the protein molecules tend to exhibit linear or circular conformation during translocation. Furthermore, by applying different types of force fields, the conformation as protein molecules pass through the channel will be affected.

Comparing to bare flow channels, the surface-modified flow channels have some unique properties, which can make a significant impact on the transport process of substances. In the simulation system of Alexeev et al., the inner surface of the bottom channel wall is lined with a regular array of rigid pillars that are inclined with respect to the flow direction (Figure 5D(a)). Each pillar is constructed using layers of seven hexagonally close-packed DPD beads. By changing the tilt angle of the pillars, we can control to better capture the polymers suspended in the flowing mixed fluid or keep them away from the flow channel wall to prevent their depositions (Figure 5D(b)). They demonstrated that this surface patterned channel can be utilized for separating colloid-polymer mixtures.

In many experimental studies, modification of the substrates has been a hot issue in scientific research. Through adjusting the shape, concentration, arrangement, tilt angle, and other factors of the decorations, we can prepare functionalized substrates with different properties (Figure 5D(c)). Figure 5E shows a polymer brush-modified cylindrical channel in experiment in which the modified polymer layer will undergo conformational changes according to the environmental pH. By changing the
pH of the environment, the width of the flow channel can be regulated. In other words, we can switch the transport process between two states, “on” and “off.”

For the biomacromolecules, such as DNA molecules and proteins,[114–120] Wang et al. reported that they can regulate the velocity of DNA transport by changing the interaction between DNA chains and the coated self-assembled monolayer (SAM).[121] As can be seen in Figure 6A, the strong interaction between the hydrophilic SAM and the DNA slows down the transport velocity of DNA in the flow channel, while the hydrophobic SAM concentrates the DNA in the center of the flow channel, accelerating the transport process. When DNA translocates through a nanometer-size pore in the ionic solution with an external electric field, the types and concentration of ions and pore diameter will affect the DNA translocation time, as mentioned already in the work of Kowalczyk and co-workers (Figure 6B) through all-atom molecular dynamics simulations.[122] Ranjith et al.[123] were able to separate DNA chains of different lengths by designing the hydrophobicity of the walls. Figure 6C demonstrated that the long DNA chains are more likely to travel to the upper half of the channel, whereas the short chains move to the lower half of the channel in most cases.

4. Summary and Outlook

DPD has increasingly become a powerful tool in solving soft matter in micro/nano channel flows, leading to a detailed insight into the structural, dynamical, and transport properties of various soft matter and the events taking place inside the fluidic channels. In this review, we have introduced the general aspect and basic formulations of DPD, and discussed how different boundary conditions based on DPD can be developed for generating wall-bounded flows, including Lees–Edwards boundary...
condition, solid wall with freezing DPD beads, and bead-layers with proper reflections. Examples were highlighted in which the models based on DPD are developed to simulate flow-induced transport through fluidic channels for some typical soft matter systems, covering red blood cells, vesicles, polymers, and biomacromolecules. Moreover, some key factors regarding the implementation of DPD method in the flow-induced transport through fluidic channels are detailed within the description of these different examples.

There are also several challenges in the aspects of further advancing the DPD technique in this exciting field. More precise boundary conditions are expected to be exploited and harnessed to simulate emerging soft matter systems with well-defined channel flows. More investigations need to be conducted on studying fundamental properties and exploring new applications of flow-induced transport of various soft matter through a fluidic channel, which is useful for current and future fluidic technologies. Particularly, with the rapidly growing ability to control the size and polydispersity of nanoscale lipid vesicles and the expanded utility of these assemblies as nanoreactors, the fundamental understanding on the transport of such small-scale vesicles and their interactions with potential payloads remains largely unresolved. In future, such a mesoscopic method must play an increasingly important role in the field of material and devise design as well as technical development based on fluidic transport of soft matter through micro/nano channels, which is also essential for understanding the transport properties of biological materials in living organisms.

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Conflict of Interest

The authors declare no conflict of interest.

Keywords
dissipative particle dynamics, flow-induced transport, micro/nano channel flow, simulation, soft matter

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