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Movement and evolution of macromolecules in a grooved micro-channel

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Abstract. This paper presented an investigation of macromolecular suspension in a grooved channel by using the dissipative particle dynamics (DPD) with finitely extensible non-linear elastic (FENE) bead spring chains model. Before studying the movement and evolution of macromolecules, the DPD method was first validated by modeling the simple fluid flow in the grooved channel. For both simple fluid flow and macromolecular suspension, the flow fields were analyzed in detail. It is found that the structure of the grooved channel with sudden contraction and expansion strongly affects the velocity distribution. As the width of the channel reduces, the horizontal velocity increases simultaneously. Vortices can also be found at the top and bottom corners behind the contraction section. For macromolecular suspension, the macromolecular chains influence velocity and density distribution rather than the temperature and pressure. Macromolecules tend to drag simple fluid particles, reducing the velocity with density and velocity fluctuations. Particle trajectories and evolution of macromolecular conformation were investigated. The structure of the grooved channel with sudden contraction and expansion significantly influence the evolution of macromolecular conformation, while macromolecules display adaptivity to adjust their own conformation and angle to suit the structure so as to pass the channel smoothly.

Keywords: dissipative particle dynamics; macromolecular suspension; grooved micro-channel

1. Introduction

Understanding the dynamic behavior of macromolecules, such as DNA, is very important for fundamental research and practical applications in bio, chemical and medical engineering, especially in designing micro-devices. Recently, micro-devices enable processing, analyzing, and delivering biochemical materials in a wide range of biomedical and biological applications (Chun *et al.* 1999, Fan *et al.* 2003). For example, micro-needle can be used to efficiently and precisely deliver a small amount of drug or DNA into local tissue, skin regions, and even cells. In order to avoid pain and tissue traumas caused by traditional technologies of drug injection and delivery, a variety of micro-needles have been designed for hypodermic injection and transdermal drug delivery (Brazzle *et al.* 1999, Lin and Pisano 1999). Micro-channels are the main field to deliver and control injected materials. By designing optimal structures of micro-channels or micro-channel networks, it is possible to efficiently control the injection process, either for simple

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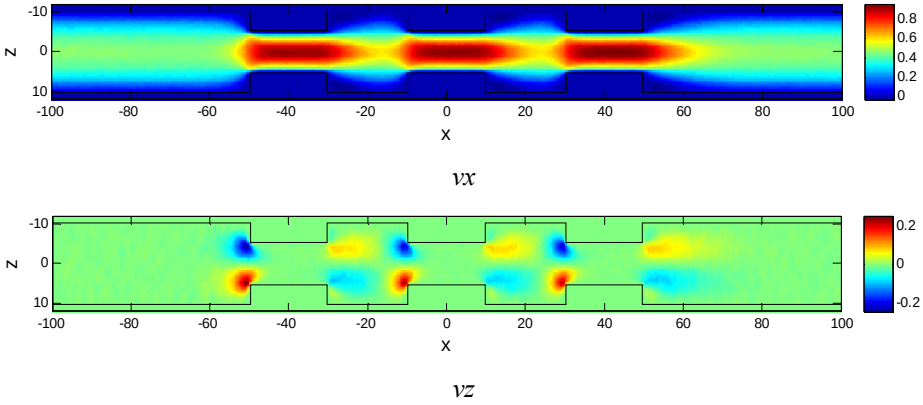

Fig. 9 Velocity field (top: horizontal velocity *vx*; bottom: vertical velocity *vz*)

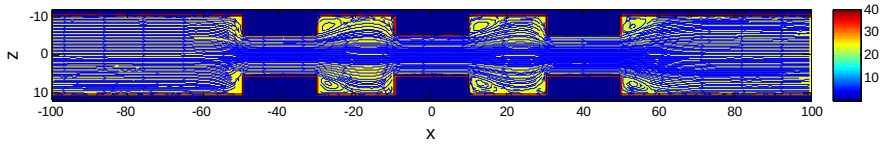

Fig. 10 Streamline of the flow field

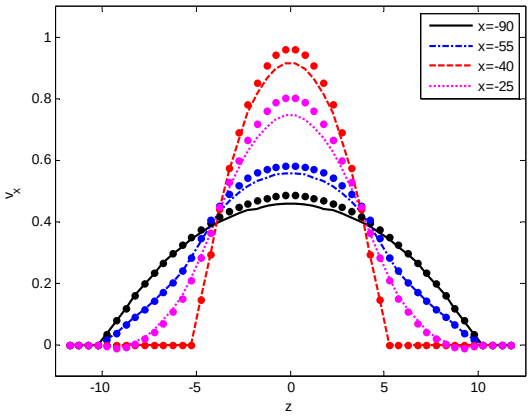

Fig. 11 Velocity, profiles at different *x*. (Dots indicate the velocity profiles of simple DPD fluid flow)

It is not easy for us to identify the difference properties between flow of macromolecules suspension and flow of simple fluid by directly observing the flow fields. Hence, we draw the profiles of horizontal velocity at x = -90, -55, -40 and -25 (see Fig. 11). In Fig. 11, lines indicate the horizontal velocity profiles from macromolecules suspension, while dots indicate those from simple fluid flow.

From Fig. 11, we can see that macromolecular chains have remarkable influences on the velocity distribution across the micro-channel. The existence of macromolecular chains will drop velocity in center region of the channel. It is observed that the impact of the macromolecular

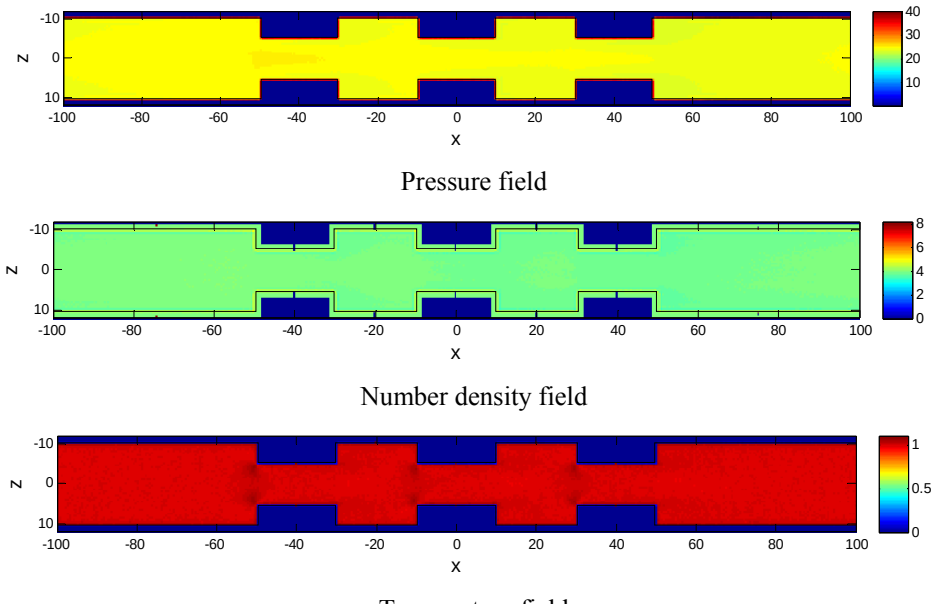

Fig. 12 Pressure (top), density (middle) and temperature (bottom) field

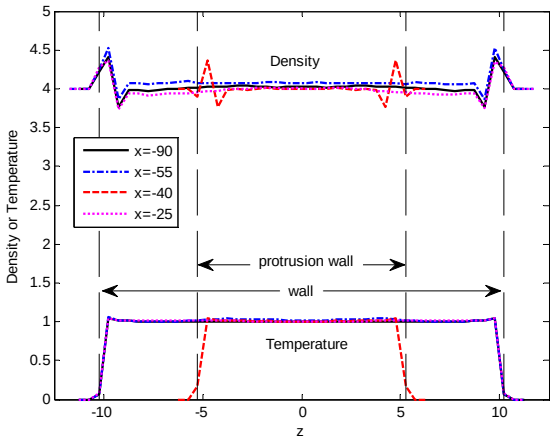

Fig. 13 Density and temperature profiles at different x across the slit

chains on the velocity distribution is more significant in the region $-5 \leq z \leq 5$, and this result is consistent with the phenomenon that most chains are distributed in the region $-5 \leq z \leq 5$ as shown in Fig. 8.

Fig. 12 shows the pressure, number density and temperature field of macromolecules suspension flow. Similar to the simple fluid flow, pressure, number density and temperature are almost uniform in the channel except for some areas close to walls.

We also draw the profiles of density and temperature at $x = -90$, -55, -40 and -25 as shown in Fig. 13. We can see the existence of macromolecule chains do not significantly influence the temperature distribution: the temperature is almost uniform across the channel and is very close to

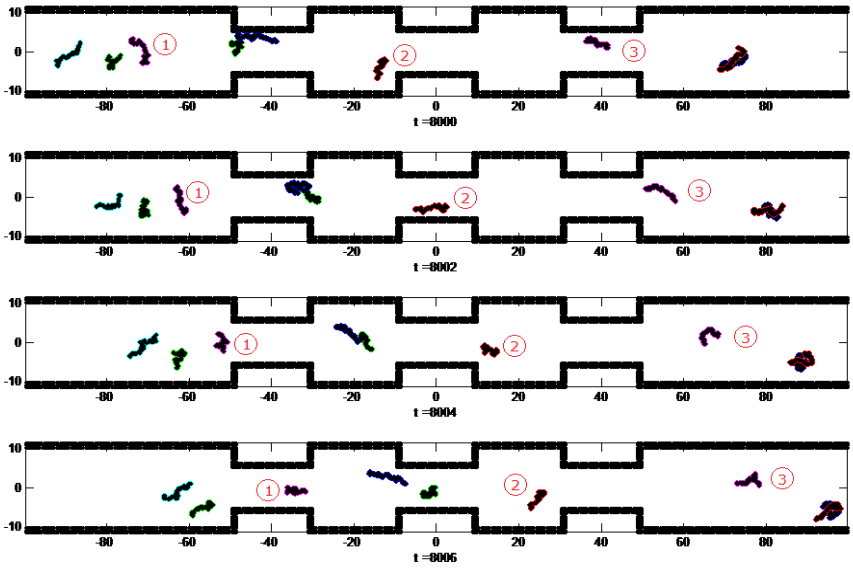

Fig. 14 Conformation evolution of marked macromolecules passing through the channel

the given temperature, but only drops near the wall due to low wall temperature. Meanwhile, macromolecular chains have slight influence on the density distribution across the micro-channel: the density of central region is slightly higher instead of uniform across the channel. Region where macromolecular chains are relatively dense has a slight higher particles density. Whether there exists macromolecules or not, a fluctuation in density exists in the regions near the wall.

In order to observe the dynamic behavior of macromolecules passing through the channel, serial frames of cconformations of marked macromolecules in the channel are plotted in Fig. 14. It is observed that macromolecules kept changing their own conformation due to the random force in DPD formula, which corresponds to the thermal fluctuations in mesoscopic scale. From the conformations of a single macromolecule in the serial frame, we can find that macromolecule trend to stretch longer when passing the region close to wall than middle region of the channel. The structure of the grooved channel with sudden contraction and enlargement affect the conformation evolution of the macromolecule significantly. To better illustrate this effect, we labeled each macromolecule in Fig. 14. When facing a sudden contraction, macromolecule tends to coil itself, or adjust the direction of extension to parallel the protruding wall, to pass the channel smoothly. For example, Macromolecule # 1 changes from a stretching state to becomecurled before and close to the contraction section. Macromolecule # 2 changes from a vertically stretching state to become a horizontal stretching state, and become curled before, in and after the contraction section. When facing a sudden enlargement, macromolecule can stretch and rotate, just as shown by Macromolecule # 3. A detailed conformation and trajectory observation of macromolecule show that there is no macromolecule trapped by the vortices inside the cavity for the whole simulation time, while simple DPD particle can be trapped by the vortices. Therefore, it is reasonable to draw such a conclusion: macromolecule would like to adjust its own conformation and angle to suit the flow and pass the channel quickly.

5. Conclusions

In this paper, we investigated the transport and conformation of macromolecules in a grooved micro-channel by using the dissipative particle dynamics model with finitely extendible non-linear elastic bead spring chains model. The grooved micro-channel is characterized by periodically placed rectangular protruding bottleneck. We firstly use the DPD model to simulate the simple fluid flow in the grooved micro-channel. The flow fields and profiles were analyzed. We found that the horizontal velocity is smaller in the region near the wall. As the width of the channel reduces, the horizontal velocity increases simultaneously. The structure of the grooved channel with sudden contraction and expansion strongly affects the velocity distribution. Vertices can also be found at the top and bottom corners behind the contraction section. The particle trajectories were also investigated by tracking four typical trajectories of particles in detail. It is found that particles can be trapped or escape from the vertices, while no particles trapped inside the cavities for the whole simulation time.

After the successful simulation of simple DPD fluid in the grooved micro-channel, we use DPD particles with FENE chains to model the movement and evolution of macromolecules in grooved micro-channel. Our numerical results show that macromolecular chains influence velocity and density distribution rather than the temperature and pressure. Macromolecular chains have remarkable influence on the velocity distribution across the channel. The existence of macromolecular chains will reduce velocity in the center region of the channel where most chains were found. Macromolecular chains have slight influences on the density distribution across the channel. The density in the central region is slightly higher instead of uniform across the channel. For regions where macromolecular chains are relatively dense, the associated particle density is slightly higher. It can be concluded that macromolecules tend to drag simple fluid particles, reducing their velocity, and leading to density and velocity fluctuations. We also analyzed the cconformation evolution of macromolecules passing through the channel, and conclude that macromolecules are able to adjust their own conformations to suit the shape of geometric structures and pass the channel smoothly.

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