

## A Simple and Effective Boundary Model in Nonequilibrium Molecular Dynamics Method<sup>\*</sup>

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**Abstract** We propose a simple and effective boundary model in a nonequilibrium molecular dynamics (NEMD) simulation to study the out-of-equilibrium dynamics of polymer fluids. The present boundary model can effectively weaken the depletion effect and the slip effect near the boundary, and remove the unwanted heat instantly. The validity of the boundary model is checked by investigating the flow behavior of dilute polymer solution driven by an external force. Reasonable density distributions of both polymer and solvent particles, velocity profiles of the solvent and temperature profiles of the system are obtained. Furthermore, the studied polymer chain shows a cross-streaming migration towards center of the tube, which is consistent with that predicted in previous literatures. These numerical results give powerful evidences for the validity of the present boundary model. Besides, the boundary model can also be used in other flows in addition to the Poiseuille flow.

**Keywords:** Boundary condition; Depletion effect; Velocity profile; Density distribution; Nonequilibrium molecular dynamics.

### INTRODUCTION

Poiseuille flow is pressure-induced flow in a long duct, like a pipe or a micro-tube. For polymer fluid, when it flows in a micro-tube driven by the external field<sup>[1]</sup>, it behaves as Poiseuille flow<sup>[2]</sup>. In recent years, many techniques have been devoted to study the nonequilibrium properties of polymer fluid under flow, one of which is the powerful nonequilibrium molecular dynamics (NEMD) method<sup>[3–6]</sup>. There are two typical methods to introduce external fields in NEMD simulations. The first one is to impose a pressure drop on the inlet and the outlet of a simulation box. This method is occasionally implemented in particle-based methods<sup>[3]</sup>, but is commonly used with a purpose of tracking down the evolution of densities, like in Lattice Boltzmann method<sup>[7, 8]</sup>. For particle-based simulations, the most popular way is to impose a constant body force on every particles in the fluid<sup>[9]</sup>. When the pressure gradient is kept constant, the aforementioned two methods have equivalent effectiveness.

The introduction of a body force will lead to a continuous increase in the velocity and temperature of the fluid. Consequently, a thermostat is normally imposed on the system to remove the redundant heat<sup>[10]</sup>. For NEMD simulations, the usually used thermostats have been illuminated clearly in some textbooks<sup>[11, 12]</sup>.

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Recently, Shirts *et al.* systematically compared the effects of different thermostats on the transport properties and kinetics of polymer solutions<sup>[13]</sup>. These thermostats can be assorted into two scenarios, *i.e.*, "velocity randomizing" thermostats and "velocity scaling" thermostats. For "velocity randomizing" thermostats, such as Andersen thermostat, a subset of particles are randomly selected and reassigned with new velocities at each time step, which are chosen from the Maxwell-Boltzmann distribution corresponding to a target temperature<sup>[13]</sup>. On the other hand, for "velocity scaling" thermostats, like Berendsen method, the velocity of each particle in the system is rescaled to a target temperature each time step, and the magnitude of velocity scaling is normally low<sup>[14]</sup>. Another kind of "velocity scaling" thermostat, like the widely used Nosé-Hoover method<sup>[11]</sup>, relaxes the instantaneous temperature of a studied system to the target temperature in an oscillatory manner by coupling to an extended system. All the aforementioned thermostats keep the studied system at a target temperature *via* adjusting the peculiar velocity of each particle, which cannot be easily captured in experiments. Even in simulations, there are some difficulties in getting the peculiar velocity of a particle, since the peculiar velocity is gained only after taking a subtraction of the streaming velocity from the laboratory velocity<sup>[9, 15, 16]</sup>, and there are more or less some artificial errors caused by the different ways to get streaming velocities<sup>[16–18]</sup>. So that in some simulations, only the velocity components in the directions orthogonal to the flow are thermostated to simplify the complexity of calculations<sup>[3]</sup>.

An alternative method to control the temperature of a given system is the wall-fluid coupling method<sup>[3, 16, 18, 19]</sup>, in which a wall takes the unwanted heat away from the fluid so that the peculiar velocity for each particle is not needed to be captured. This method has a more realistic analog, like a bath in experiments. For NEMD simulations, the wall can be modeled by several rows of wall particles, and it can also be described as a boundary condition following the specular-diffuse reflection law. The wall-fluid coupling method is popular in non-equilibrium studies<sup>[16, 19, 20]</sup>, where the wall is composed of thousands of wall particles arranged in several layers of (100), (111) or (110) face-centered cubic (fcc) structures<sup>[16, 20]</sup>. The wall particles either have fixed positions with infinite mass, or vibrate around the initial positions *via* a spring potential<sup>[20]</sup>. Numerical results indicated that the wall density and the lattice plane of the wall particles had significant impact on the characteristics of the nanochannel flow<sup>[19, 20]</sup>. There was a large depletion layer near the boundary and the fluid density oscillated strongly<sup>[17, 21]</sup> due to the interaction between the wall particles and fluid particles. Besides, in some cases, the velocity profiles had totally an upward shift, and then the effective radius of the tube was enlarged attributed to the slip effect, *i.e.*, the polymer fluid particles near the boundary wall have relative velocities against the wall<sup>[3, 20]</sup>.

Inspired by the aforementioned reports, in this work we are intended to reduce the effect of the wall and remove the unwanted heat when dealing with non-equilibrium systems. We propose a simple and effective boundary model to study the out-of-equilibrium fluid by using NEMD simulation. The boundary model is composed of hundreds of movable wall particles moving in the wall region of the tube. The validity of the boundary model is tested by investigating the flow behavior of a polymer fluid driven by an external force. Numerical evidences certify that our boundary model is very effective in controlling velocity, density and temperature profiles. The detailed description of the boundary model is given in model and simulation details, and the validity of this boundary model is shown in results and discussion.

## MODEL AND SIMULATION DETAILS

The validity of our boundary model is investigated by studying the flow behavior of a polymer fluid driven by an external force and confined in a tube, which has a radius of  $R_p = 5.8\sigma$  and a length of  $L = 24.36\sigma$  (as shown in Fig. 1). The tube wall is comprised of hundreds of wall particles whose particle number density is  $\rho_w = 1.25(1/\sigma^3)$  (The tube walls with  $\rho_w$  in a range of  $1.20(1/\sigma^3)$ – $1.30(1/\sigma^3)$  have similar validity). There is Lennard-Jones potential  $U_{LJ}(r)$  among each two wall particles with  $\epsilon_{ww} = 1.0\epsilon$ .

$$U_{LJ}(r) = \begin{cases} 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right] & r < r_c \\ 0 & r \geq r_c \end{cases} \quad (1)$$

where  $r$  is a distance between interacting particles. For convenience,  $\sigma$ ,  $\epsilon$  and monomer mass  $\mu$  are used as units of length, energy and mass, the time is measured in unit of  $\tau_{LJ} = (\mu\sigma^2/\epsilon)^{1/2}$ , and the cutoff diameter  $r_c$  is  $2.5\sigma$  in reduced units<sup>[22]</sup>.

The wall particles move in the wall region of the tube, which has an inside radius of  $R_p = 5.8\sigma$  and an outside radius  $R_0$ , as shown in Fig. 1,  $R_0 = R_p + \delta_w$ , where  $\delta_w = 0.9\sigma$ . The periodic boundary condition is employed in the  $x$ -direction along the axial direction of the tube. In the  $y$ -direction or  $z$ -direction (two orthogonal directions along the radial direction of the tube), a simple bounce-back condition is used to keep the wall particles moving in the wall region, *i.e.*, if a wall particle gets out of the boundary region at the position of  $r_d = R_p$  or  $r_d = R_0$  ( $r_d$  is the distance apart from the center of the tube) in an integration step, it will be bounced back to its original position by a reversed velocity<sup>[23]</sup>.

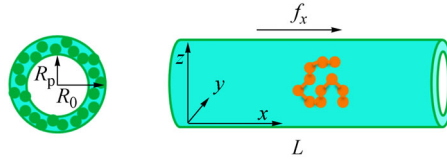


**Fig. 1** A sketch of the boundary model (The online version is colorful.)

For the polymer and solvent particles, whose particle number density is selected to be  $\rho = 0.82(1/\sigma^3)$ <sup>[24, 25]</sup>, there are Lennard-Jones potentials with  $\epsilon_{ff} = 1.0\epsilon$  embodying excluded volume interaction among each two polymer monomers or solvent particles. The polymer and solvent particles are subject to the periodic boundary condition in  $x$ -direction. In the other two directions, Lennard-Jones potentials between wall particles and fluid particles with  $\epsilon_{fw} = 1.0\epsilon$  are used to maintain the polymer and solvent particles moving inside of the tube. The bounce-back condition is used in the  $y$ -direction or  $z$ -direction to prevent any polymer or solvent particles entering the boundary region in some extreme cases.

The single polymer chain has a length of  $N = 30$ . It is described as a single bead-spring chain which can be considered as a freely jointed chain<sup>[26]</sup>. The solvent is taken to be athermal for the polymer chain. Neighboring monomers interact with each other *via* finitely extensible nonlinear elastic (FENE) potential  $U_{FENE}(r)$ .  $U_{FENE}(r)$  is given as follows,

$$U_{FENE}(r) = -\frac{k}{2} R_0^2 \ln \left( 1 - \frac{r^2}{R_0^2} \right) \quad (2)$$

where the spring constant  $k$  is set as  $k = 7.0\epsilon/\sigma^2$ , and the ultimate bond length  $R_0$  is  $2.0\sigma$  in reduced units<sup>[27]</sup>.

In this system, the polymer fluid flows driven by an external force. The driving force  $f_x$  is imposed on the polymer fluid in the  $x$ -direction. The motion of polymer monomers, solvent particles and wall particles follows the governing equations<sup>[11, 28]</sup>,

$$\dot{r} = \frac{p}{m} \quad (3)$$

$$\dot{p} = -\frac{\partial U}{\partial r} \quad (4)$$

$$\dot{p} = -\frac{\partial U}{\partial r} + f_x \quad (5)$$

which are integrated by using Verlet-Velocity algorithm<sup>[29]</sup> with an integration time step of  $\delta t = 0.004 \tau_{LJ}$ . Verlet-cell list method is used to improve the computational efficiency<sup>[11]</sup>. Meanwhile, we employ Nosé-Hoover thermostat to control the temperature of the wall particles, whose target temperature is  $k_B T_0 = 1.0 \varepsilon$ . Via heat exchange between wall particles and polymer fluid particles, the redundant heat is removed from the polymer fluid. To obtain a steady flow, we first relax the studied system for a period of relaxation of  $1.0 \times 10^6$  time steps. After that, we collect and discuss the data obtained in the following  $8.0 \times 10^6$  time steps.

## RESULTS AND DISCUSSION

### The Temperature Profiles of Polymer Fluids

In our model, the polymer fluid is driven by an external force  $f_x$  in a range of  $0.017 \varepsilon/\sigma$ – $0.73 \varepsilon/\sigma$ , which in turn generates viscous heat. In Poiseuille flow, the viscous heat is inhomogeneous due to the fact that the viscous heat is proportional to the square of the local strain rate<sup>[15]</sup>. The inhomogeneity of viscous heat will lead to a local heat flux, which is predicted by Fourier's law<sup>[15]</sup>. Solving the Navier-Stokes equation in the weak-flow limit, we can obtain the temperature profile  $T(r) \sim T_c + T_f r^{\alpha_T}$ , where  $\alpha_T$  is 4.0 for Poiseuille flow,  $T_c$  is the temperature averaged over the particles in the circular bin with a width of  $0.3\sigma$  nearest the wall,  $r$  is the distance apart from the center of the tube, and  $T_f$  is a parameter relevant to the driving force  $f_x$ <sup>[15]</sup>. We first focus on the distribution of temperature of the studied polymer fluid. Figure 2 gives the temperature profiles of the system, where each point in the curves is obtained based on a statistic average over the speeds in  $y$  and  $z$  directions of polymer and solvent particles in the same circular bin with a width of  $0.5\sigma$ <sup>[18]</sup>. The temperature profiles in Fig. 2 are similar with the classical fourth-order temperature profile generated by viscous heating in Poiseuille flow. The temperatures  $T_c$  are listed in Table 1.  $T_c$  is very close to the target temperature in the system with a weak driving force  $f_x$ . However, when  $f_x$  becomes relatively strong,  $T_c$  increases, but the curve of  $T/T_c$  still shows a quartic profile (As listed in Table 1, when the driving force is  $f_x = 0.73 \varepsilon/\sigma$ , the exponent  $\alpha_T$  is 4.12, which is quite close to 4.0 predicted by Navier-Stokes equation). This suggests that the temperature profile is reasonable by using the present boundary model.

### The Velocity and Density Distributions of Polymer Fluids

In the weak-flow limit, a velocity profile of  $V_x(r) \sim V_{x0} + V_2 r^{\alpha_v}$  with  $\alpha_v = 2.0$  is obtained by solving the Navier-Stokes equation for Poiseuille flow, where  $V_{x0}$  is the streaming velocity of polymer fluid at the tube center, and  $V_2$  is a parameter relevant to the external force  $f_x$ <sup>[15]</sup>. The above expression can be rearranged as  $V_x(r) \sim V_{x0} [1 - (r/R_{pe})^{\alpha_v}]$ , where  $R_{pe}$  is the effective radius of the tube. In our work, the velocity distribution in the radial direction of the tube is illustrated in Fig. 3. The streaming velocity  $V_x$  of each data point in Fig. 3 is obtained via an average of the  $x$ -direction speeds of particles in the bin box of  $0.5\sigma \times 0.5\sigma$ <sup>[30]</sup>. The exponents  $\alpha_v$  are obtained and listed in Table 1 by power-law fitting the velocity profiles.  $\alpha_v$  is in the range of 1.72–2.07, which is relatively close to the exponent 2.0 of a parabolic velocity profile for Poiseuille flow<sup>[30, 31]</sup>. The effective tube radii  $R_{pe}$  (also listed in Table 1) are in the range of  $5.69\sigma$ – $5.75\sigma$ , which are quite close to the initial setting  $R_p = 5.8\sigma$ . This implies that the slip effect and depletion effect are weakened by using our boundary model.

The density profiles of the polymer fluid further illuminate the reduction of the depletion layer, as shown in Fig. 4. The solvent density profiles in Fig. 4(a) exhibit two distinct regions: a bulk-like region of uniform density in the central region of the tube and an interfacial region near the tube wall<sup>[17]</sup>. In the interfacial region, the particles layer is in the radial direction of the tube, and the layered structure gradually disappears at a distance of about  $3\sigma$  from the tube wall. The fluctuation of  $\rho_s/\rho$  for the present boundary model is much smaller than the stiff harmonic spring wall particle model<sup>[17]</sup>, where the fluctuation near the wall is larger than 2.0. If the external force  $f_x$  gets relatively strong, the amount of solvent particles in the bulk-like region will decrease due to the increase of temperature in this region (shown in Fig. 2), which is consistent with previous work<sup>[17]</sup>. Moreover, the solvent particles in our model can be much closer to the tube wall, due to the fact that the value of  $\rho_s/\rho$  is higher than 0.5 at a distance of  $0.4\sigma$  from the tube wall, so the depletion effect near the boundary is effectively weakened. Therefore, the reasonable velocity and density profiles imply that the present boundary model can be used to investigate the flow behaviors of the microfluids under Poiseuille flow.

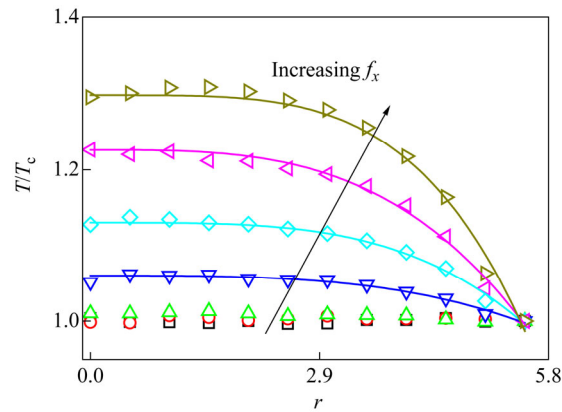


**Fig. 2** The temperature profiles of polymer fluids driven by different forces  $f_x = 0.017$  ( $\square$ ),  $0.075$  ( $\circ$ ),  $0.15$  ( $\triangle$ ),  $0.29$  ( $\nabla$ ),  $0.44$  ( $\diamond$ ),  $0.58$  ( $\triangleleft$ ) and  $0.73$  ( $\triangleright$ ) ( $T_c$  is the temperature of the bin nearest the wall,  $r$  is the distance apart from tube center. The solid lines are the corresponding fitting lines with temperature profile curve  $T(r) \sim T_c + T_f r^{\alpha_T}$ .) (The online version is colorful.)

**Table 1.** The values of  $T_c$ ,  $R_{pe}$ ,  $\alpha_T$  and  $\alpha_V$  for the polymer fluids driven by different external forces  $f_x$

| $f_x$ | $k_B T_c$ | $\alpha_T$ | $R_{pe}$ | $\alpha_V$ |
|-------|-----------|------------|----------|------------|
| 0.017 | 1.00      | —          | —        | —          |
| 0.075 | 1.00      | —          | —        | —          |
| 0.15  | 1.02      | —          | 5.70     | 2.07       |
| 0.29  | 1.08      | 3.40       | 5.74     | 1.78       |
| 0.44  | 1.18      | 3.70       | 5.75     | 1.74       |
| 0.58  | 1.34      | 3.28       | 5.72     | 1.77       |
| 0.73  | 1.54      | 4.12       | 5.69     | 1.72       |

$T_c$  is the temperature averaging over the particles nearest the wall,  $R_{pe}$  is the effective tube radius, and  $\alpha_T$  and  $\alpha_V$  are the exponents of temperatures and velocity profiles, respectively.

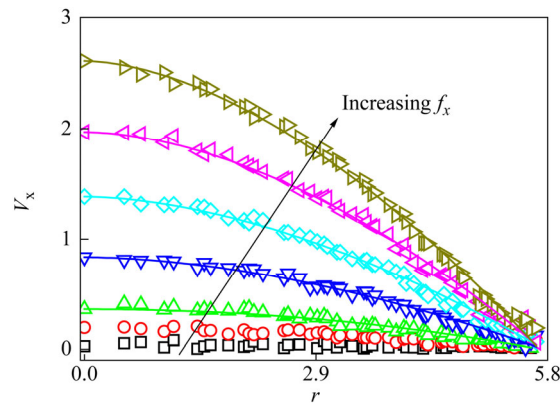


**Fig. 3** The velocity profiles of polymer fluids driven by different external forces  $f_x$  in a range of  $0.017\sigma \sim 0.73\sigma$

The solid lines are the corresponding fitting lines with  $V_x(r) \sim V_{x0} + V_2 r^{\alpha_V}$ , and the symbols have the same meaning as in Fig. 2. (The online version is colorful.)

Figure 4(b) gives the density profiles of the polymer chain subjected to different driving force  $f_x$ . Obviously,  $\rho_p/\rho$  increases in the bulk-like region and decreases in the interfacial region with increasing  $f_x$ . This result indicates that the increasing external force makes the polymer chain have a cross-streaming migration towards the center of the tube. Furthermore, we collect statistics for the position distribution  $P_d$  of mass center of the

studied polymer chain driven by different external forces  $f_x$  over thousands of samples, and show them in Fig. 5. A clear cross-streaming migration towards the center of the tube is observed. The occurrence of a migration towards the tube center is caused by the hydrodynamic interaction between the polymer chain and the tube wall. The stronger the external force is, the closer the polymer chain gets to the tube center<sup>[32]</sup>. This result is consistent with that reported in recent literatures<sup>[31, 33]</sup>.

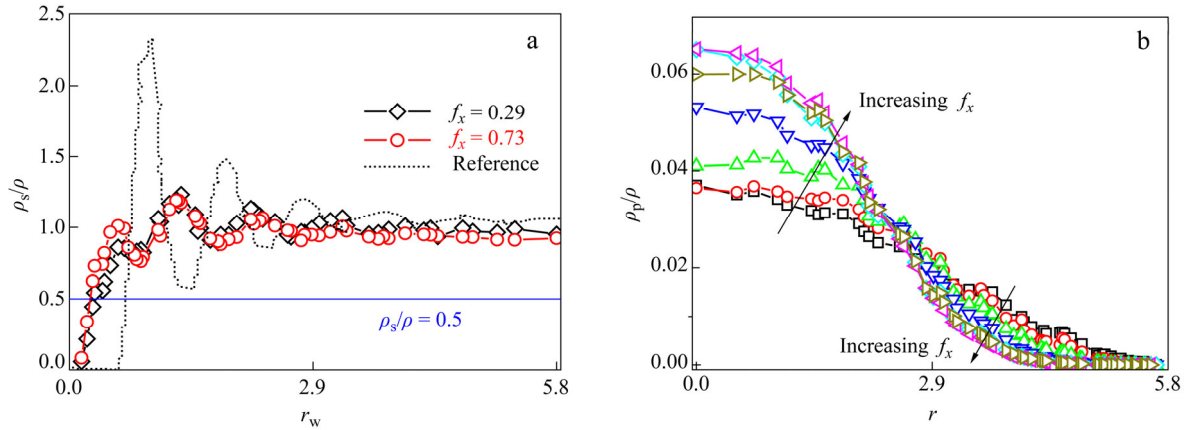


**Fig. 4** (a) The density profiles for the solvent particles when the external forces  $f_x = 0.29\epsilon/\sigma$  ( $\diamond$ ) or  $0.73\epsilon/\sigma$  ( $\circ$ ), where  $r_w$  is the distance apart from the boundary (The dashed line comes from Khare's results<sup>[17]</sup> and the blue line is a guideline for  $\rho_s/\rho = 0.5$ ); (b) The density profiles for the polymer monomers with different external forces  $f_x = 0.017$  ( $\square$ ),  $0.075$  ( $\circ$ ),  $0.15$  ( $\triangle$ ),  $0.29$  ( $\nabla$ ),  $0.44$  ( $\diamond$ ),  $0.58$  ( $\triangleleft$ ) and  $0.73$  ( $\triangleright$ ) ( $r$  is the distance apart from the center of tube.) (The online version is colorful.)

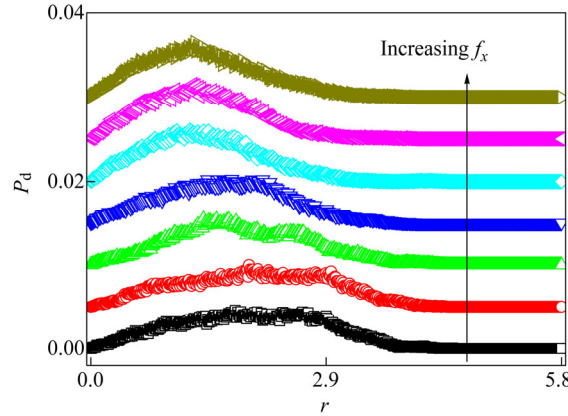


**Fig. 5** The position distributions of the mass center of polymer chain plotted as functions of  $r$  ( $r$  is distance apart from the tube center. All the data points are shifted upward with an interval of 0.005 for better visualization.) (The online version is colorful.)

### The Orientation Dependence on External Forces for the Polymer Chain

Another interesting issue is the orientation of the polymer chain under flow. The orientation of a polymer chain can be characterized by the probability distribution functions  $P(\theta)$  and  $P(\varphi)$  as functions of the orientation angles  $\theta$  and  $\varphi$ <sup>[34–36]</sup>, where  $\theta$  is the angle between the polymer end-to-end vector and its projection onto the  $xy$  plane, and  $\varphi$  is the angle between the projection and the flow direction<sup>[34]</sup> (A sketch of angles  $\theta$  and  $\varphi$  is shown in Fig. 6a). Figures 6(b) and 6(c) show the probability distribution functions  $P(\theta)$  and  $P(\varphi)$ , respectively. Obviously, the external force induces the polymer chain orientating quickly, even for a very weak driving force ( $f_x = 0.017\epsilon/\sigma$ ), and the orientation effect is strengthened with increasing  $f_x$ . This can be found from the increase

of  $P(\theta < 0.5)$  in Fig. 6(b) and  $P(-0.5 < \varphi < 0.5)$  in Fig. 6(c). This result means, in most cases, the single polymer chain tends to orientate along the direction of the external force, as reported by Redding *et al*<sup>[31]</sup>.

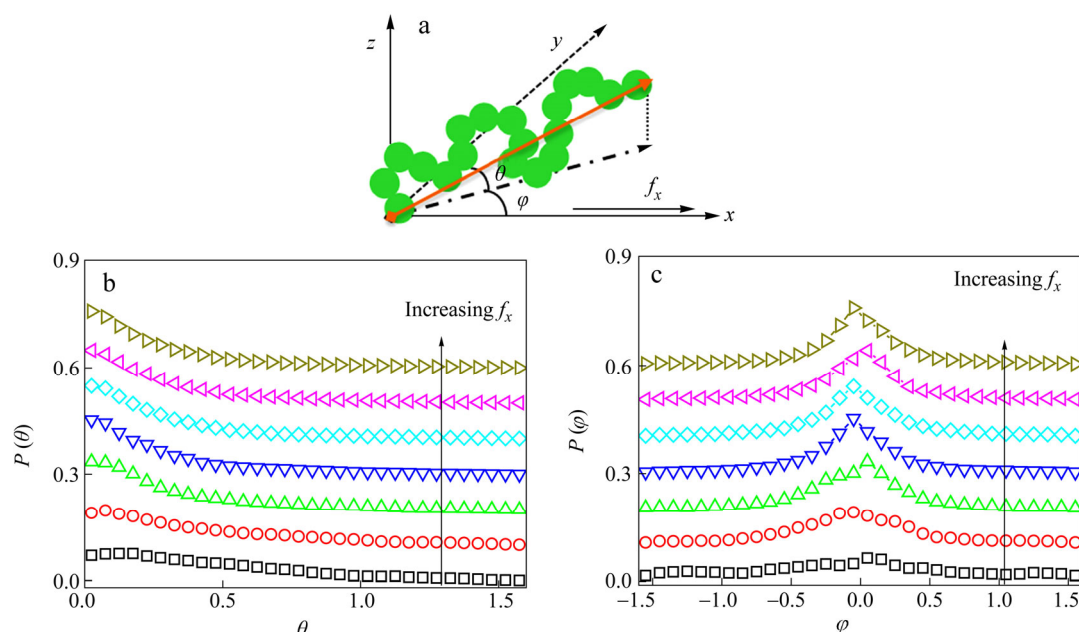


**Fig. 6** (a) A sketch of  $\theta$  and  $\varphi$ , the probability distribution functions  $P(\theta)$  (b) and  $P(\varphi)$  (c) of the orientation angles  $\theta$  and  $\varphi$  for the polymer chain (Similar to Fig. 5, the data points in (a) and (b) are shifted upward with an interval of 0.1 for better visualization.) (The online version is colorful.)

## CONCLUSIONS

We have proposed a simple and effective boundary model to study the out-of-equilibrium dynamics of polymer fluids by using nonequilibrium molecular dynamics method. We have investigated the flow behaviors of polymer fluids undergoing Poiseuille flow by using the present boundary model. The numerical results show that the polymer fluids have reasonable temperature, velocity and density profiles under driving force. Furthermore, the polymer chain orientates along the flow direction and cross-streaming migrates toward the center of the tube, which are consistent with the reports of Refs.<sup>[15, 16, 20]</sup>. These aforementioned numerical studies suggest the validity of the present boundary model.

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## REFERENCES

- 1 Liu, D., Cui, K., Huang, N., Wang, Z. and Li, L., *Sci. China Chem.*, 2015, 58: 1570
- 2 Sussman, D.M., Tung, W.S., Winey, K.I., Schweizer, K.S. and Riggleman, R.A., *Macromolecules*, 2014, 47: 6462
- 3 Barrat, J.L. and Bocquet, L., *Phys. Rev. Lett.*, 1999, 82: 4671
- 4 He, Z. and Zhou, J., *Carbon*, 2014, 78: 500
- 5 ClarkII, J.K. and Paddison, S.J., *Phys. Chem. Chem. Phys.*, 2014, 16: 17756
- 6 Hu, C., Bai, M., Lv, J., Wang, P., Zhang, L. and Li, X., *Microfluid Nanofluid*, 2014, 17: 581
- 7 Succi, S., "The lattice boltzmann equation for fluid dynamics and beyond", Clarendon Press, Oxford, 2001

- 8 Kekre, R., Butler, J.E. and Ladd, A.J., Phys. Rev. E, 2010, 82: 011802
- 9 Todd, B.D. and Daivis, P.J., Molecular Simulation, 2007, 33: 189
- 10 Ouyang, Y., Hao, L., Ma, Y. and Guo, H., Sci. China Chem., 2015, 58: 1013
- 11 Allen, M.P. and Tildesley, D.J., "Computer simulation of liquids", Clarendon: Oxford, 1987
- 12 Frenkel, D. and Smit, B., "Understanding molecular simulation: from algorithms to applications", Academic Press, 2002
- 13 Basconi, J.E. and Shirts, M.R., J. Chem. Theory Comput., 2013, 9: 2887
- 14 Berendsen, H.J.C., Postma, J.P.M., van Gunsteren, W.F., DiNola, A. and Haak, J.R., J. Chem. Phys., 1984, 81: 3684
- 15 Todd, B.D. and Evans, D.J., Phys. Rev. E., 1997, 55: 2800
- 16 Todd, B.D., Evans, D.J. and Daivis, P.J., Phys. Rev. E, 1995, 52: 1627
- 17 Khare, R., de Pablo, J. and Yethiraj, A., J. Chem. Phys., 1997, 107: 2589
- 18 Heinbuch, U. and Fischer, J., Phys. Rev. A, 1988, 40: 1144
- 19 Thompson, P.A., Nature, 1997, 389: 360
- 20 Soong, C.Y., Yen, T.H. and Tzeng, P.Y., Phys. Rev. E, 2007, 76: 036303
- 21 Varnik, F. and Binder, K., J. Chem. Phys., 2002, 117: 6336
- 22 Fu, C., Sun, Z. and An, L., Chinese J. Polym. Sci., 2013, 31(3): 388
- 23 Li, Z.Q., Li, Y.J., Wang, Y.M., Sun, Z.Y. and An, L.J., Macromolecules, 2010, 43: 5896
- 24 Dünweg, B. and Kremer, K., J. Chem. Phys., 1993, 99: 6983
- 25 Fu, C., Ouyang, W., Sun, Z. and An, L., J. Chem. Phys., 2007, 127: 044903
- 26 Underhill, P.T. and Doyle, P.S., J. Non-Newtonian Fluid Mech., 2004, 122: 3
- 27 Fu, C., Sun, Z. and An, L., J. Phys. Chem. B, 2011, 115: 11345
- 28 Fu, C., Jia, X., Sun, Z. and An, L., Polymer, 2014, 55: 4538
- 29 Rappaport, D.C., "The art of molecular dynamics simulation", Cambridge university press, 1997
- 30 Koplik, J., Banavar, J.R. and Willemsen, J.F., Phys. Rev. Lett., 1988, 60: 1282
- 31 Reddig, S. and Stark, H., J. Chem. Phys., 2011, 135: 165101
- 32 Sekhon, G., Armstrong, R.C. and Jhon, M.S., J. Polym. Sci., Part B: Polym. Phys., 1982, 20: 947
- 33 Ma, B.H. and Graham, M.D., Phys. Fluids, 2005, 17: 083103
- 34 Huang, C.C., Sutmann, G., Gompper, G. and Winkler, R.G., Europhys. Lett., 2011, 93: 54004
- 35 Winkler, R.G., Phys. Rev. Lett., 2006, 97: 128301
- 36 Gerashchenko, S. and Steinberg, V., Phys. Rev. Lett., 2006, 96: 038304