Hydrodynamic effects on flow-induced polymer translocation through a microfluidic channel

Xuejin Li a,b,*, Igor V. Pivkin c,d,**, Haojun Liang b,e,***

a Division of Applied Mathematics, Brown University, Providence, RI 02912, USA
b CAS Key Laboratory of Soft Matter Chemistry, Department of Polymer Science and Engineering, University of Science and Technology of China, Hefei, Anhui 230026, People’s Republic of China
c Institute of Computational Science, Faculty of Informatics, University of Lugano, Lugano 6904, Switzerland
d Swiss Institute of Bioinformatics, Lausanne 1015, Switzerland
e Hefei National Laboratory for Physical Sciences at Microscale, University of Science and Technology of China, Hefei, Anhui 230026, People’s Republic of China

Article info
Article history:
Received 17 April 2013
Received in revised form 1 June 2013
Accepted 11 June 2013
Available online 20 June 2013

Keywords:
Polymer translocation
Hydrodynamic interaction
Computer simulation

ABSTRACT
The flow-induced translocation of polymer chains through a microfluidic channel is investigated using particle-based Dissipative Particle Dynamics and modified Langevin Dynamics approaches. Adaptive no-slip wall boundary conditions have been implemented to model fluid flow in the microfluidic channel, paying attention to controlling fluid density fluctuations. By varying the magnitude of the external body force driving the flow, an extensive simulation study of the dynamics of flow-induced translocation of polymers with and without considering hydrodynamic interactions (HIs) was performed. The results show that the HIs can increase the translocation probability and reduce the translocation time. In addition, the results also demonstrate that the solid wall interfacial property exerts a considerable influence on the dynamics of polymer translocation, i.e., an attractive interaction between the solid wall and the polymer increases the translocation time, whereas a repulsive interaction decreases it.

1. Introduction
The translocation of polymers through narrow channels is a ubiquitous process in nature. Important examples include RNA transport through nuclear pores, viral injection of DNA into host cells, and protein transport into mitochondria, chloroplasts and across the vessel walls in healthy and tumor induced microcirculation. The translocation of polymers through narrow channels can also lead to several potentially industrial and technical applications, including rapid DNA sequencing, genomic partitioning techniques and information storage on macromolecules. It is not surprising that the translocation of polymers has received increasing attention in experimental [1–4], theoretical [5–7], and computational studies [8–13], because of its broad applications in many fields and its importance for understanding fundamental processes in biology and polymer sciences. During the translocation processes of polymers through the narrow channels, the number of available configurations of polymers decreases, resulting in an effective entropic barrier for polymers. Therefore, an external driving force such as an external electric field [14–18], chemical potential gradient [19], pressure gradient [20–23], adsorption potential [24], solvent selectivity difference [18,25], or a direct pulling force [26,27], is needed to overcome the entropic barrier and hasten the translocation.

Despite considerable interest in the problem, minimal attention has been paid to effects of the hydrodynamic interactions (HIs) on the dynamics of polymer translocation [28–32]. Recent Lattice Boltzmann (LB) [29,31] and molecular dynamics (MD) [33] results have shown that the HIs may have considerable influence on polymer translocation processes. For example, Lehtola et al. carried out a set of simulations of biopolymer translocation through a narrow channel and got a power-law scaling relationship between the average translocation time and the biopolymer chain length [31]. The exponent values obtained in their simulations varied

---

* Corresponding author. Division of Applied Mathematics, Brown University, Providence, RI 02912, USA.
** Corresponding author. Institute of Computational Science, Faculty of Informatics, University of Lugano, Lugano 6904, Switzerland.
*** Corresponding author. CAS Key Laboratory of Soft Matter Chemistry, Department of Polymer Science and Engineering, University of Science and Technology of China, Hefei, Anhui 230026, People’s Republic of China.
E-mail addresses: Xuejin_Li@brown.edu (X. Li), igor.pivkin@usi.ch (I.V. Pivkin), hjliang@ustc.edu.cn (H. Liang).

0032-3861/$ – see front matter © 2013 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.polymer.2013.06.022
between 1.05 and 1.13 with hydrodynamics and between 1.25 and 1.52 without hydrodynamics. An acceleration in polymer translocation in the presence of the HIs was obtained by Pyta et al. [29], whereas Hernández-Ortiz et al. found that the hydrodynamic forces accelerate or hinder translocation of polymers depending on their molecular weight [32]. The effect of the HIs on the dynamics of DNA translocation has been studied by Izmítili et al. [34], but they found that the HIs play only a minor role in the dependence of the translocation time on DNA chain length.

The studies described above considered the effect of hydrodynamics on forced polymer translocation mainly driven by a direct pulling force. An applied pressure gradient, which generates a fluid flow in a microfluidic channel, can also drive polymers through the narrow channel [35,36]. For example, the flow-induced polymer translocation in computational research has been studied by Marksteijn et al. [35], who found that the translocation probability is independent of the polymer chain lengths. This observation is in consistent with previous theoretical results that the critical suction current in linear polymers is independent of the degree of polymerization [37]. A similar phenomenon that the translocation is independent of polymer chain length for short chains has been observed in Brownian Dynamics (BD) simulations of electrophoresis [38,39]. Nikoubashman and Likos [36] have also recently studied the translocation of linear and branched polymers through narrow and patterned channels driven by Poiseuille flow. They have confirmed the independence between the translocation probability and the polymer and dendrimer lengths and found that the threshold flux is slightly higher in dendrimers than that in linear polymers. Despite the fact that the translocation of polymers in narrow channels has been studied for many years, several important aspects of fluid flow field as a translocation mechanism remain unexplored, requiring a more fundamental study of the flow-induced polymer translocation. Such studies could lead to better understanding of the microfluidic channel transport of polymers and the effect of hydrodynamic forces and interactions during the polymer translocation. Dynamic simulations and modeling helped to predict how polymer behaves in fluidic flows and channels [40,41]. An insight into the details of flow behaviors of individual polymers taking place in complex microfluidic channels is required to understand the role of the HIs in the translocation processes of polymers.

Dissipative Particle Dynamics (DPD) and Langevin Dynamics (LD) (or BD) methods are two powerful computer simulation techniques to study the large-scale dynamics of polymers and colloids in dilute solution. The DPD method, which is a coarse-grained particle-based simulation technique in three dimensions and correctly represents the HIs, has been successfully applied to study a wide variety of complex hydrodynamic phenomena ranging from simulating vesicle formation in block copolymers [42–44] to modeling the rheological properties of blood flow [45–47]. The LD method is an approach to the mathematical modeling of the dynamics of molecular systems, and the BD method is a simplified version of the LD method and corresponds to the limit where no average acceleration takes place during the simulation run. The LD (or BD) scheme neglects the effect of the HIs which may exist in a real system [48,49]. To capture correctly the dynamics of the polymers and colloidal particles and reproduce experimental results, the HIs must be included in LD (or BD) algorithms. In past decades, the LD (or BD) algorithms which incorporate the HIs have been successfully employed to simulate polymer and colloidal dynamics in dilute solutions and in flows [50–52].

We present extensive simulations of the flow-induced translocation of polymers through a microfluidic channel both in the presence and in the absence of HIs. We employ two coarse-grained particle-based simulation methods, i.e., the DPD and the LD methods. The polymer architecture, connectivity, interactions, and the solvent compressibility are explicit in both methods. The difference between the two is that the HIs are taken into account in the former method, but they can be absent in the latter one [48,49]. Thus, we can isolate and study the effect of HIs in the presence of all other physical effects. The rest of the paper is organized as follows.

In Section 2 we briefly introduce the simulation methods. In Section 3 we describe the particle-based model. Our numerical results are presented and discussed in Section 4. Finally, in Section 5 we summarize the findings and present the conclusions.

2. Simulation method

We study the flow-induced translocation of polymers with the help of DPD and LD simulation techniques. Both methods describe the same Hamiltonian system but differ in the evolution algorithm. In DPD simulations [53–55], particles \( i \) and \( j \) at positions \( r_i \) and \( r_j \) interact with each other via soft pairwise forces, which are given by:

\[
F^D_{ij} = a_{ij} \omega(r_{ij}) \mathbf{n}_{ij},
\]

\[
F^D_{ij} = -\gamma \omega^2(r_{ij}) (\mathbf{n}_{ij} \cdot \mathbf{v}_{ij}) \mathbf{n}_{ij},
\]

\[
F^D_{ij} = \sigma \omega(r_{ij}) \zeta \Delta t^{-1/2} \mathbf{n}_{ij},
\]

where \( r_{ij} = r_i - r_j, r_{ij} = |r_{ij}|, \mathbf{n}_{ij} = r_{ij}/r_{ij}, \) and \( \mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j \). The coefficients \( a_{ij}, \gamma \) and \( \sigma \) define, respectively, the strength of conservative (\( F^D_{ij} \)), dissipative (\( F^D_{ij} \)) and random (\( F^R_{ij} \)) forces. In our DPD simulations, the values of \( \gamma \) and \( \sigma \) are equal to 4.5 and 3.0, respectively. In addition, \( \zeta \) is a random number with zero mean and unit variance. The weight function \( \omega(r_{ij}) \) is given by

\[
\omega(r_{ij}) = \begin{cases} 1 - r_{ij}/r_c, & r_{ij} < r_c, \\ 0, & r_{ij} \geq r_c. \end{cases}
\]

where \( r_c \) is the cutoff radius, which gives the extent of the interaction range. In the DPD method, the dissipative force and the random force act as heat sink and source respectively. Combined, the two forces acts as a thermostat that keeps the mean temperature of the system constant. Another contribution of these two forces is that they conserve momentum locally, so that hydrodynamic modes of the fluid emerge even for small particle numbers.

In LD simulations [56], particles also interact with each other via pairwise conservative force given by Eq. (1), whereas the dissipative and random forces act relative to a fixed background as

\[
F^D_i = -\gamma \mathbf{v}_i,
\]

\[
F^R_i = \sigma \zeta \Delta t^{-1/2},
\]

where \( \mathbf{v}_i \) is the velocity vector of particle \( i \). In the LD (or BD) method, each particle experiences a random force independently of all other particles; thus, this scheme neglects the effect of the HIs. For details on the LD (or BD) method and the absence of the HIs, we refer to Refs. [48,49].

Following previous computational studies [57–59], the coefficient of the repulsive force between two alike particles is set to \( a_{ij} = 25.0 \) for \( i = F, S, W \), causing the simulated compressibility of these particles at room temperature to correspond to the experimental value. As suggested by Nardai and Zifferera [60], we have the expectation that \( a_{PS} \leq 25.0 \) for good solvent condition, \( a_{PS} = 27.2 \) for \( \theta \) solvent condition, while \( a_{PS} \geq 30.0 \) for bad solvent
condition. Thus, a manipulation of relative wall–polymer interactions enables us to explicitly introduce net-attractive or repulsive wall forces on the polymer. In this study, the repulsive parameter between the polymer and wall particles is set at $\alpha_{NW} = 25.0$ to represent the neutral wall case. For the cases of attractive and repulsive walls, we chose the values $\alpha_{NW} = 17.5$ and 32.5. The parameters used in simulations are listed in Table 1.

An external body force is applied to each fluid particle to generate a fluid flow in the microfluidic channel. In present study, the external body force is of the form,

$$f^\text{ext}_i = g z_i,$$

where $g$ is the magnitude of the body force, and $z_i$ is a vector unit in the flow direction. To avoid the overlap of particles and to remove density fluctuations in the simulation domain, we include a Morse force for interactions between pairs of particles, which has the form,

$$F_{ij}^M = 2D_x \beta \left[ e^{\beta(2r_i-r)} - e^{\beta(2r-r_i)} \right] \mathbf{n}_{ij},$$

where $D_x = 500.0$ and $r_i = 0.32r_c$ are the well depth and rigid core radius of the Morse potential, and $\beta = 0.5$ characterizes the interaction range.

Following the mapping strategy in our previous study [22], we obtain the length scale $r_c = 1.12$ nm and time scale $t_r = 0.21$ ms. The simulations are performed using a modified version of the atomistic code LAMMPS [61]. The equations of motion are integrated using a modified velocity-Verlet algorithm with $\lambda = 0.50$ and time step $\Delta t = 0.004 t_r$. Typical simulation takes about $5.0 \times 10^6$ time steps.

3. Simulation model

3.1. System geometry and solid wall boundary conditions

The model geometry we consider throughout this study, as illustrated in Fig. 1, has an inlet and an outlet. A wide channel of circular cross-section with a length $L = 50.0r_c$ and a diameter $D = 20.0r_c$ is on the left side of the microfluidic system. The wide channel tapers into a narrow channel with a length $l = 10.0r_c$ and a diameter $d = 4.0r_c$. The right half of the microfluidic system is a mirror image of the left half. Periodic boundary conditions are used in the $z$ direction, while the flow is bounded by solid walls in other directions.

In fluid dynamics, the fluid velocity at fluid-solid boundary is always equal to that of the solid boundary, thus, the no-slip condition is used almost universally in modeling of fluid flows [62]. As with most engineering approximations, the no-slip condition does not always hold in reality; for example, a non-zero slip length has been observed in some highly hydrophobic surfaces [63,64]. Thus, one needs to impose the slip boundary condition in simulations of these phenomena. Actually, in recent years, a number of MD and DPD studies have examined factors that determine the magnitude of the slip length at liquid–solid interfaces [65–74]. On the other hand, when one performs DPD simulation of Poiseuille flow in a microchannel, the soft repulsion between two particles cannot prevent fluid particles from penetrating solid boundaries, and thus extra effort is required to impose the no-slip boundary condition [75].

Interaction of liquids with solid walls causes layering of the fluid, which is responsible for the large density fluctuations near the wall. These fluctuations are physical and thus desirable in simulations, but they may be erroneous in some other simulations [75]; for example, spurious density fluctuations have been observed in particle systems such as stochastic rotational dynamics [76], MD [77] and DPD simulations [78]. Thus, one needs to control the density fluctuations in wall-bounded DPD systems.

In order to enforce the no-slip boundary condition at the fluid–solid interface, we employ an adaptive boundary condition model [75,78]. At the pre-equilibrium stage, the computational domain covers both fluid and solid wall regions and is assumed to be periodic in all directions. The hydrostatic simulation is run until the equilibrium state is reached, resulting in a homogeneous particle density in the system. Particles located inside the solid wall region are then frozen to model walls in combination with bounce-back reflections at the fluid–wall interface to prevent the penetration of polymer/fluid particles into the solid walls. An adaptive force is applied to fluid particles in the vicinity of the walls in order to control fluid density fluctuations near the solid walls [78]. The magnitude of the force depends on the distance of the fluid particles to the solid walls and is dynamically updated during the simulations according to the estimated density fluctuations. In all of the following simulations, the no-slip wall boundary is implemented to model the fluid flow with zero velocity at fluid–solid boundary, and the adaptive boundary condition is employed to control the particles’ density fluctuations in microfluidic channel.

3.2. Polymer model

In our simulations, the polymer is modeled as a linear bead-spring chain with the Finitely Extensible Nonlinear Elastic (FENE) potential. Two consecutive monomers in polymer chain interact with each other via the FENE potential,

$$U_F^{\text{FENE}} = -\frac{k_s}{2} r_{\text{max}}^2 \log \left[ 1 - \frac{r^2}{r_{\text{max}}^2} \right]$$

where $r_{\text{max}} = 0.75r_c$ is the maximum spring extension between consecutive monomers and $k_s = 100.0$ is the spring constant. When the distance between two connected monomers approaches $r_{\text{max}}$, the spring attractive force increases to infinity, and therefore the length greater than $r_{\text{max}}$ is not allowed. Besides, each monomer in the polymer chain is also subject to the standard DPD or LD forces described by Eqs. (1)–(6).

<table>
<thead>
<tr>
<th>Table 1</th>
<th>Repulsion parameter sets used in polymer–solvent–wall interaction calculations.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wall property</td>
<td>$\alpha_{WP}$</td>
</tr>
<tr>
<td>Neutral</td>
<td>25.0</td>
</tr>
<tr>
<td>Attractive</td>
<td>25.0</td>
</tr>
<tr>
<td>Repulsive</td>
<td>25.0</td>
</tr>
</tbody>
</table>

Fig. 1. Schematic representation of the simulation model for polymer chain and microfluidic channel. In this figure, the blue, green and gray particles represent the fluid, polymer and wall particles, respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)
total of 97,500 fluid particles with a particle number density of 3.0. The equilibrated radius of gyration of polymer with the longest chain length \( N = 400 \) is approximate to \( R_g^2(0.5) \approx 4.94r_c \); therefore, an estimated value of \( 2(R_g^2)^{0.5} \approx 9.88r_c \) is obtained for the polymer size with the longest chain length \( N = 400 \). The diameter of the wide and narrow cylindrical channels are \( d = 20.0r_c \) and \( 4.0r_c \). Thus, the polymer size with the longest chain length is more than twice the diameter of the narrow cylindrical channel; while it is less than half the diameter of the wide cylindrical channel. The polymer monomers are initially placed randomly on the left side of the wide channel, far from the entrance to the narrow channel. This is different from most simulation cases of polymer translocation, where one end of polymer is initially placed at the entrance of the channel. Thus, the polymer, to a certain extent, moves freely in the microfluidic channel. After the polymer chain is equilibrated, an external body force is applied to the fluid particles, while the polymer chain is fixed at the equilibrated position until a steady fluid flow in the narrow channel is obtained. We subsequently release the polymer chain, and the fluid flow carries the polymer chain through the narrow channel.

We monitor the instantaneous position of each polymer monomer during the translocation processes. The translocation time is measured from the moment when one or several polymer monomers enter into the narrow channel, to the moment when the entire polymer chain passes through the narrow channel. In case when the part of the polymer chain that initially has entered the narrow channel ejects back to the left side of the narrow channel, the translocation time needs to be measured again when the polymer chain re-enters the narrow channel. The translocation process is considered to be successful when the polymer traverses the narrow channel from its left end to the right end. We have performed the simulations with totally independent initial conformations until at least 500 successful translocation events were obtained. The statistics over the successful translocation events were then evaluated, neglecting the failed runs.

## 4. Results and discussion

### 4.1. Simulation method validation

We model the polymer translocation through the microfluidic channel using particle-based DPD and LD simulation techniques. To validate the results, first a simple fluid flow (without polymers) in a straight microfluidic channel of diameter \( D = 20.0r_c \) is simulated at external body force \( g = 0.5 \). Fig. 2 shows comparison of the simulation results with the corresponding theoretical solution. The velocity profiles extracted along the cross-flow (\( x \)-axis) direction for DPD and LD simulations are shown in Fig. 2(a) and (b), respectively. In Fig. 2(a), zero velocities at the solid walls as well as parabolic velocity profiles are observed. From the theoretical solution, we get the velocity \( v_x = gD^2/8\eta = 11.96 \times [1 - (x/10)^2] \). The DPD results agree well with the theoretical solution. In the absence of the HIs, a uniform flow is expected to develop. The fluid velocity in the cross-flow direction can be obtained via \( v_z = g/\gamma = 0.111 \). In

---

**Fig. 2.** (a) Velocity profiles of pure fluid flow in the cross-flow direction of the straight microfluidic channel with considering the HIs. (b) Velocity profiles of pure fluid flow in the cross-flow direction of the straight microfluidic channel without considering the HIs between fluidic particles. (c) Velocity profiles of the particle-based simulation (atomistic) results and the Navier–Stokes solutions (continuum) obtained for the center plane of microfluidic channel at different stations. The simulation results are extracted at: Location A \((z = -3.0r_c, \text{before the narrow channel})\), Location B \((z = 0.0r_c, \text{middle of the narrow channel})\), and Location C \((z = 3.0r_c, \text{after the narrow channel})\). (d) Particle density profiles in the cross-flow direction of the fluid flow. Solid line represents the input value of the particle number density. The distance between the dash lines represents the width of the narrow channel.
the LD simulations without considering the HIs, a uniform velocity profile in the cross-flow direction is obtained, see Fig. 2(b). The results also agree well with the theoretical solution.

To better understand the hydrodynamic effects in the polymer translocation and compare the simulation results in the same flow conditions, we use a modified LD method. In the modified LD model, we adopt standard LD dissipative and random forces described by Eqs. (5) and (6) for polymer—polymer, polymer—fluid, polymer—wall interactions, whereas we keep the conventional DPD dissipative and random forces as in Eqs. (2) and (3) for fluid—fluid and fluid—wall interactions. This approach allows to obtain a parabolic velocity profile in the cross-flow direction, while the HIs between the polymer and polymer/fluid/wall particles are absent. In the presence of the HIs, the polymer molecule traverses along the flow direction by the external flow field; Without considering the HIs, the polymer can also moves and diffuses slowly because of the collisions of the flowing fluid particles.

To verify the accuracy of the simulation results for the fluid flow in the particular microfluidic channel shown in Fig. 1, we then simulate a fluid flow (without polymer) in the microfluidic channel and compare results with a numerical Navier–Stokes solution, which is obtained using the (continuum-based) spectral element simulation solver NEKTAR. Fig. 2(c) shows the velocity profiles extracted along the cross-flow (x-axis) direction at several different locations for LAMMPS (atomicistic) and NEKTAR (continuum) solutions. In this figure, zero velocities at the solid walls as well as quasi-parabolic shapes of the velocity profiles are noticed. There are no visible differences between the atomicistic and continuum results. Fig. 2(d) shows the density profiles for fluid particles obtained in the simulations. Although small difference in density profiles along the microfluidic channel is present, the deviations are quite small. The density profiles extracted perpendicular to the flow direction are also uniform, apart for statistical fluctuations. Thus, the fluid flow can be accurately modeled using these modified approaches. Therefore, to establish the effects of the HIs, a comparison can be made by performing the simulations in the same microfluidic channel with tunable hydrodynamics, while keeping all other simulation parameters the same. Moreover, to allow comparison with other studies using different polymer models and simulation methods, we calculate the Peclet number, which is defined as the ratio of convective velocity of the flow to thermal velocity of DPD particles [79] and has the form,

\[ Pe = Re · Sc = \frac{D < V_x >}{\eta_d}, \]

where \( D \) is the diffusivity and \( < V_x > \) is the average velocity of the fluid particles. In the following sections, we analyze the simulation results with the Peclet number.

### 4.2 Translocation probability

The translocation of polymer through the microfluidic channel is carried out under the hydrodynamic flow field. Basically, there are three stages in the translocation process of linear polymer molecules: (1) approach; (2) activation; and (3) translocation [39].

First, we calculate polymer attempt time, \( \tau_{\text{att}} \), which is characterized by the average time it takes for a polymer monomer located at the entrance to insert itself into the narrow channel divided by the time to find the polymer monomer at the entrance to the narrow channel [80]. The functional dependence of \( \tau_{\text{att}} \) with the polymer chain length \( N \) is shown in Fig. 3(a). We find that \( \tau_{\text{att}} \) decreases non-linearly with polymer chain length, which indicates that shorter polymer chains take more time to travel to the entrance of the narrow channel. A shorter \( \tau_{\text{att}} \) for a longer polymer chain could result from it larger size because parts of the longer polymer chain may lie simultaneously in areas of weak and strong fluid flow field. Thus, part of the polymer chain which lie in areas of strong fluid flow field are driven toward the entrance of the narrow channel, resulting in the entire chain moving there.

Without the HIs, there is an upward shift in the \( \tau_{\text{att}} \sim N \) curves, which indicates that the polymer chains take more time to move to the entrance of the narrow channel. In order to provide a more quantitative account, we measure the distribution of the attempt time both in the presence and in the absence of the HIs. The histogram of \( \tau_{\text{att}} \) at polymer length \( N = 200 \) and Peclet number \( Pe = 80 \) is shown in Fig. 3(b). We find that the distribution of \( \tau_{\text{att}} \) is close to a Gaussian distribution in the presence of the HIs, whereas it is asymmetric with a long exponential tail in the absence of the HIs. One possible reason is that in the presence of the HIs, the fluid particles can affect and effectively control the velocities of polymer monomers. For the polymer translocation in the absence of the HIs, this regulatory effect does not exist, resulting in larger fluctuations of polymer monomers during the process.

As mentioned in Section 3.2, we refer to a successful translocation as the event when the polymer chain fully traverses the narrow channel from the left-side of it to the right-side. Otherwise, the translocation is considered to be unsuccessful. It is interesting to investigate the translocation probability in the polymer
translocation process. The translocation probability, denoted as \( P(N) \), is then computed as the fraction of simulations leading to effective successful translocation events that one or several polymer monomers have entered the narrow channel without first exiting. Fig. 4 shows \( P(N) \) as a function of the polymer chain length, \( N \), at \( P_e \approx 80 \) with and without considering the HIs. We find that \( P(N) \) decreases with \( N \) from a large value near 1 to a small value close to zero. We attribute the changes to the mismatch between the polymer size and the pore size of the narrow cylindrical channel. For a longer polymer chain, the polymer size is larger than the diameter of narrow cylindrical channel, thus, the polymer chain undergoes continuous attempts to shorten its size in the cross-flow direction to fulfill complete translocation. In addition, there is a slight decrease in the trend in probability of translocation in the absence of the HIs compared to that for polymers in the presence of the HIs. This finding is considered to be reasonable as there is a wider range of polymer fluctuation in the absence of the polymer—fluid hydrodynamics coupling. Compared to that in simulations with the HIs, the probability that the polymer exits the narrow channel due to fluctuations is greater, thus, reducing the probability of successful translocation.

4.3. Scaling behavior between the average translocation time and polymer chain length

The dynamics of polymer translocation through the microfluidic channel is described by its translocation time, \( \tau \). Fig. 5(a) shows the scaling relationship between the average \( \tau \) and the length of the polymer chain \( N \) with and without considering the HIs. Two different regimes for the average translocation time dependence on the polymer length are observed. That is, \( \tau \) is independent of \( N \) in short polymers, while there is a scaling relation with \( \tau \sim N^{\beta} \) for longer polymers. A polymer length is considered to be critical if its value is approximately \( N \approx 75 \) in the current study, as we keep the diameter of the narrow channel fixed. The polymer chain of length \( N < 75 \) does not need, or needs only slightly, to change its shape to traverse the narrow channel, therefore the translocation time is almost constant for \( N < 75 \). For longer polymer chains with \( N > 75 \), we obtain a power-law scaling of \( \tau \sim N^{\beta} \) with an exponent equal to \( \beta = 1.20 \pm 0.04 \) in the presence of the HIs, whereas \( \beta \) increases to \( 1.33 \pm 0.03 \) in the absence of the HIs.

A more direct means of tracking the translocation process of polymer is given by observing the variation in the radius of gyration of polymer, \( \langle R_g^2 \rangle \), with the time development. Fig. 5(b) shows that the polymer clearly has a large conformational deformation during the translocation; however, there is only a slight increase in \( \langle R_g^2 \rangle \) during the approach process, i.e., the process from the time that polymer chain is released to the time that part of polymer chain first contacts with the pore. Thus, in our opinion, the reduction of the entropic barrier to translocation is small and the translocation time is dominated by the external fluid flow field. Subsequently, there is an increase in radius of gyration of polymer, which indicates that polymer chain elongate its size in the flow direction. \( \langle R_g^2 \rangle \) then increases dramatically until it reaches the maximum, implying that the polymer chain is extended and stretched by the hydrodynamic flow field during translocation.

In addition, when the polymer chain length is very large, the average translocation time, \( \tau \), increases rapidly. This may be related to the polymer chain entanglement during the translocation process. The fluid particles are modeled explicit in the present study, and the polymer is in a crowded fluid particle environment. Thus, it may be difficult for the polymer to change its configuration for traversal through the narrow channel, since part of the polymer chain already inside the narrow channel is constrained.

4.4. Influence of the solid walls

Polymer depletion and cross-streamline migration phenomena in microfluidic channels are important in microfluidic devices and a variety of biological systems. These effects might be relevant in physical processes such as polymer adsorption, lubrication, and transport. For flow-induced translocation of polymer in a microfluidic channel, the polymer is stretched by the fluid velocity...
gradient. Due to the asymmetric streamlines around an extended polymer chain near the solid walls, the polymer migrates from the solid walls towards the channel centerline, leading to polymer depletion near the solid walls. In the simulations presented above, the interactions between the polymer—fluid and polymer—wall as well as polymer—polymer are identical, i.e., a neutral solid wall for which no explicit adsorption or repulsion is expected during the polymer translocation. However, solid walls, in general, can induce adsorption or repulsion of polymers, the polymer monomers are thus either attracted or repelled by the solid wall interface, resulting in different translocation dynamics of polymer.

It is of fundamental and practical interest to study the transport of polymer chain within the microfluidic channel under the influence of the solid wall interfacial property. One quantity which can be used to characterize the location of the polymer chain inside the microfluidic channel is the center-of-mass probability distribution, \( P(x) \), across the channel. To describe non-equilibrium transport phenomena in polymer system, we performed simulations with 50 statistically independent initial conformations. Each simulation was carried until at least 20 successful translocation events were obtained. The combination of multiple trajectories and long simulation times provided us with smooth \( P(x) \), even though only one polymer chain was present in the simulation domain.

Variation of relative interactions between polymer-, wall- and fluid-particles allows us to explicitly introduce attractive or repulsive wall forces on the polymer. By adding an attractive interaction

\[
\begin{align*}
\text{(a)} & \quad \text{(b)} \\
\text{(c)} & \quad \text{(d)} \\
\text{(e)} & \quad \text{(f)}
\end{align*}
\]

Fig. 6. The center-of-mass probability distribution of polymer chain, \( P(x) \), close to Location A \((z = -30.0, \text{ before the narrow channel})\) in simulations with different solid walls, with (a) and without (b) considering the HIs. Translocation time, \( t \), as a function of external body force, \( g \), in simulations with different solid walls in the presence (c) and in the absence (d) of the HIs. (e) Functional dependence of the probability of translocation of polymer, \( P(N) \), through the microfluidic channel on polymer chain length, \( N \), in neutral and attractive walls. In the figure, \( x_{c} \) represents the distance between the center-of-mass of polymer and the center of the microfluidic channel.
between polymer and solid wall particles, one can expect that it is possible to push the polymer toward the wall and thereby slow down its translocation. Here, simulations for polymers with chain length \( N = 200 \) at several different Peclet number ranged from \( Pe = 0 \) to 400 have been carried in the study. In Fig. 6(a), we show \( P(x) \) as a function of the distance \( x \) from the center of the microfluidic channel at \( Pe = 80.0 \). The polymer chain in simulations with the attractive wall exhibits smaller depletion compared to that in simulations with the neutral wall. Fig. 6(c) shows the average translocation time as the function of Peclet number in the case of neutral and attractive wall. Our results confirm that the attractive polymer–wall interaction increases the translocation time.

The simulation results with the repulsive wall show larger near-wall depletion compared to neutral and attractive walls, thus, the polymer tends to have preferred position closer to the center of the microfluidic channel. In Fig. 6(a), we also present \( P(x) \) obtained in simulations with the repulsive wall. Here, the bimodel distribution is more pronounced. The consequence being that the polymer chain has a higher average velocity and, therefore, reduced translocation time (see Fig. 6(c)). A quite remarkable speedup is evident. The HIs between the polymer monomers and solid walls are crucial for the observed bimodel distribution and depletion layer near the solid walls. In Fig. 6(b), we show \( P(x) \) obtained in simulation with different solid walls in the absence of the HIs. In contrast with results shown in Fig. 6(a), the bimodel distribution and the minimum in the centerline disappear, whereas the depletion layer close to the solid walls is less pronounced. It even decreases when we change the solid walls from neutral to attractive. As a result, the polymer needs a longer time to traverse the microfluidic channel, as shown in Fig. 6(d). Next, we calculate the translocation probability for polymers with chain length ranged from \( N = 25 \) to 400 in attractive walls in the presence of the HIs, see Fig. 6(e). The figure shows that a slight increase in the trend in probability of translocation of polymers in attractive walls compared to that for polymers in neutral walls, which means that attractive walls increase the translocation probability.

The polymer adsorption in flowing fluids has recently received increasing interest for experiments [81,82], theory [83–85] and computer simulations [85–89]. The translocation of polymer through a pore or a channel can be induced by selective adsorption [24 90] or is relevant in polymer adsorption process, especially when one includes the wall repulsive or attractive effects. Using the particle-based PD and LD approaches, it would be possible to investigate the adsorption phenomena within the scope of the current study. We will investigate the adsorption phenomena in flow-induced polymer translocation in future studies.

5. Conclusions

In this paper, we have studied the effects of hydrodynamic interactions (HIs) on the flow-induced polymer translocation through a microfluidic channel. The adaptive no-slip wall boundary conditions were used in simulations to model the fluid flow in the microfluidic channel and control the fluid density fluctuations near the solid walls. The results show that the HIs can increase the translocation probability and accelerate the translocation processes. The results also show that the translocation of polymer chains through the microfluidic channel exhibits two different regimes depending on the length of the polymer chain. For polymer chains of length above the threshold, the polymer translocation process depends on the length of the polymer chain and a power-law scaling relationship \( \tau \sim N^\beta \) is obtained, where \( \beta = 1.20 \pm 0.04 \) when considering the HIs and \( \beta = 1.33 \pm 0.03 \) without considering the HIs. However, when polymer length is lower than the critical value, we find that the polymer translocation process is independent of \( N \). In the latter case, the polymer size is comparable to the size of the narrow channel, so the polymer chain does not need, or needs only slightly, to change its shape to traverse the narrow channel, thus, the average translocation time is independent of the number of monomers in the polymer chain.

We further find that it takes different time for polymer to traverse through the microfluidic channel with different solid wall interfacial property. In simulations with an attractive interaction between the polymer and solid walls, the polymer chain is found to be pushed toward the side walls and thereby the translocation process is slowed down. While the polymer chain tends to have preferred position closer to the center of the microfluidic channel in simulations with a repulsive wall, resulting in a quite remarkable speedup of the translocation process.

These findings demonstrate that particle-based Dissipative Particle Dynamics and Langevin Dynamics methods are effective (and relatively simple) simulation techniques that can be used for understanding the conformational and dynamic behaviors of polymer and DNA molecules during the translocation processes.

Acknowledgments

This work is supported by the National Natural Science Foundation of China (Grants 21004059 and 91127046), the National Basic Research Program of China (Grant 2012CB821500), and the Fundamental Research Funds for the Central Universities (Grant KC206020002). I.P. gratefully acknowledges support of Swiss National Science Foundation (Grant 200021_138231) and Swiss National Supercomputer Center (Grants s311 and s340).

References

[46] X. Li et al. / Polymer 54 (2013) 4309–4317