



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



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## 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.

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## 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

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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 Fyta 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 Izmitli 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 Markesteijn 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:

$$F_{ij}^C = a_{ij}\omega(r_{ij})\mathbf{n}_{ij}, \quad (1)$$

$$F_{ij}^D = -\gamma\omega^2(r_{ij})(\mathbf{n}_{ij}\cdot\mathbf{v}_{ij})\mathbf{n}_{ij}, \quad (2)$$

$$F_{ij}^R = \sigma\omega(r_{ij})\zeta_{ij}\Delta t^{-1/2}\mathbf{n}_{ij}, \quad (3)$$

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

$$\omega(r_{ij}) = \begin{cases} 1 - r_{ij}/r_c & r_{ij} < r_c \\ 0 & r_{ij} \geq r_c \end{cases}, \quad (4)$$

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

$$F_i^D = -\gamma\mathbf{v}_i, \quad (5)$$

$$F_i^R = \sigma\zeta_i\Delta t^{-1/2}, \quad (6)$$

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  $a_{ij} = 25.0$  ( $i = P, S, W$ ), 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

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