Effects of Electrostatic Interactions on the Translocation of Polymers Through a Narrow Pore Under Different Solvent Conditions: A Dissipative Particle Dynamics Simulation Study

Xuejin Li,* Xiaolong Li, Mingge Deng, Haojun Liang*

Polymer translocation through a narrow pore is investigated using a particle-based dissipative particle dynamics (DPD) method. A rigid core is included in each particle to avoid particle interpenetration problems based on the original DPD method. Electrostatic interactions of charged particles are simply represented via screened Coulombic interactions. The average translocation time $t$ versus polymer length $N$ satisfies the scaling law $t \sim N^{\beta}$. The scaling exponent $\beta$ depends on solvent quality. The results demonstrate that solvent quality exerts a considerable influence on the dynamics of translocation of polymers. The findings may help facilitate understanding of the dynamic behaviors of various polymer and DNA molecules during translocation processes.

1. Introduction

The dynamics of polymer translocation through a narrow pore is significant in understanding several chemical and biological processes, such as the motion of DNA and RNA molecules across nanoscopic pores, infection of viruses into the cell nucleus, and transport of proteins through membrane channels. The translocation of polymer molecules through a narrow pore 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 become a subject of intensive experimental,[1–7] theoretical,[8–16] and computational studies[17–23] because its broad applications in many fields and its importance for understanding fundamental processes in biology and polymer sciences.

The number of available configurations of polymers decreases during polymer translocation through a narrow pore, resulting in an effective entropic barrier for polymer molecules. Therefore, an external driving force, such as an external electric field,[1,4,18] a chemical potential gradi-
carried out a set of experiments on double-stranded DNA relationship with state narrow pores; they obtained a different scaling translocation of individual DNA molecules through solid-experiments. Wanunu et al. studied the voltage-driven polymer. [30] Luo et al. used molecular dynamics (MD) and polymer chain length of the average translocation time of polymer translocation. Of particular interest is the effect of solvent quality on the translocation of polymers depending on their molecular weight. [43] The effect of solvent quality on biased polymer translocation was studied by Kapakhne et al. [26] who found that the β depends on the quality of solvent. Lörcher et al. recently studied the translocation of polymers through a narrow pore induced by a bad solvent; they obtained β = 1.10. [27] In our previous simulations, we studied the dynamics of flow-induced polymer translocation through a fluidic channel under good solvent conditions. We found that the average τ versus N satisfied τ ∼ N^{1.15}. [45] Despite these previous studies, the effect of solvent quality on forced polymer translocation remain unexplored; thus, more fundamental studies on forced translocation of polymers through narrow pores are necessary. Such studies may deepen the understanding of the conformational changes and yield new results regarding the dependence of β on solvent quality during forced polymer translocation processes.

The significant role of EIs in determining the ion current on ion transport through an αHL channel has been demonstrated by Misakian and Kasianowicz. [46] This electrostatic force is expected to play a similar role during the translocation of charged polymers through narrow pores. Experimental investigations have shown that the translocation process is quite complex and highly stochastic. The experimental challenge makes the translocation of polymers an ideal target for theoretical and computational studies. In recent years, theoretical and computational studies have seen remarkable advances in charged polymer translocation through narrow pores, yet these studies have neither settled the different scaling relationships of τ with N nor established the role of EIs on charged polymer translocation. [34,47]

We present an extensive simulation study on the translocation of polymers through a narrow pore with HIs incorporation. Our interest lies in the scaling behavior between the average τ and N in the presence and absence of EIs under different solvent conditions. We employ the
dissipative particle dynamics (DPD) method, which is a continuum simulation technique in three dimensions that correctly represents hydrodynamic interactions.[48] In the past decade, the DPD method has been successfully applied to study the effects of solvent quality on the conformational and dynamical behaviors of polymers. For example, Kong et al. have employed the DPD method to study the effects of solvent quality on the conformational and relaxation of polymer molecules.[49] As the effects of solvent quality on the transport properties of polymers through membranes.

The rest of this work is organized into topics. In the next section, we describe the simulation method and employed DPD model whereas in the following section, results will be presented and discussed. Finally, we summarize the findings and present the conclusions.

2. Model Development and Simulation Method

2.1. Dissipative Particle Dynamics Formulation

We study the translocation of polymers with the help of dissipative particle dynamics simulation technique. DPD is a relatively new mesoscopic method that describes clusters of molecules moving together in a Lagrangian fashion subject to soft quadratic potentials. As a particle-based mesoscopic method, DPD considers $N_p$ particles, and the inter-particle force exerted on particles $i$ in our simulations is given by

$$
F_i = \sum_{i\neq j} \left( F^C_{ij} + F^D_{ij} + F^S_{ij} + F^M_{ij} + F^DH_{ij} + F^S_{ij} \right) + F^\text{ext}_i \tag{1}
$$

where the first three terms are the conservative, dissipative, and random forces used in a standard and original DPD simulation, which are given by

$$
F^C_{ij} = a_{ij} \omega(r_{ij}) n_{ij} \tag{2}
$$

$$
F^D_{ij} = -\gamma \omega^2(r_{ij})(\mathbf{n}_{ij} \cdot \mathbf{u}_{ij}) n_{ij} \tag{3}
$$

$$
F^S_{ij} = \sigma \omega(r_{ij}) \zeta_{ij} \Delta t^{-1/2} n_{ij} \tag{4}
$$

where $r_{ij} = r_i - r_j$, $\mathbf{r}_{ij} = |\mathbf{r}_{ij}|$, $n_{ij} = r_{ij}/r_{ij}$, and $u_{ij} = u_i - u_j$. The coefficients $a_{ij}$, $\gamma$, and $\sigma$ define, respectively, the strength of conservative, dissipative, and random forces. In the current study, the values of $\gamma$ and $\sigma$ are equal to 4.50 and 3.00, respectively, therefore, the temperature is kept at $k_B T = 1.00$. In addition, $\zeta_{ij}$ is a random number with zero mean and unit variance. The weight function $\omega(r_{ij})$ is given by

$$
\omega(r_{ij}) = \begin{cases} 
1 - r_{ij}/r_c & r_{ij} < r_c \\
0 & r_{ij} \geq r_c 
\end{cases} \tag{5}
$$

where $r_c$ is the cutoff radius, which gives the extent of the interaction range. In the DPD method, the dissipative and random forces act as heat sink and source, respectively, and the combined effect of the two forces acts a thermostat, which conserves momentum and thus provides the correct description of hydrodynamics to the system.

To avoid the particle interpenetration problem, as suggested by Nikunen et al.[52] and by Liu et al.,[53] we adopt a segmental repulsion model and a mixed hard-soft potential to each DPD particle by modifying the form of the conservative force based on the original DPD method. In the present study, the modified conservative force is approximated by the Morse force when the distance between two DPD particles, $r_{ij}$, is less than the preset rigid core diameter $2.00 r_p$, which is given by,

$$
F^M_{ij} = 2D_e \omega \left[ e^{2\omega(2r_0 - r_{ij})} - e^{\omega(2r_0 - r_{ij})} \right] n_{ij} \tag{6}
$$

where $D_e = 200.00$ is the well depth of the Morse potential, and $\omega = 0.50$ characterizes the interaction range.

The rest of the contributions in Equation 1 correspond to forces due to bonding stretching, EIs, and the external applied driving force, respectively. The bond stretching is defined by a harmonic force used to connect two consecutive particles in polymer chains. This contribution is expressed as

$$
F^b_{ij} = k_{\text{bond}} (1 - r_{ij}/r_0) n_{ij} \tag{7}
$$

where $k_{\text{bond}} = 100.00$ and $r_0 = 0.60$ are, respectively, the spring constant and equilibrium bond length between two consecutive particles.

The total force can also have an electrostatic contribution, which is derived from the electrostatic field solved by Debye-Hückel analytical method. For simplicity, the EI in the current study is represented by a screened Coulombic interaction,[22] which has the form,

$$
F^\text{DH}_{ij} = q_i q_j |\mathbf{r}_{ij}| \exp(-\kappa |\mathbf{r}_{ij}|) \frac{1}{r_{ij}} \tag{8}
$$

where $q_i$ and $q_j$ are the charges on two charged particles $i$ and $j$. The Bjerrum length $l_B = e^2/k_BT \kappa$ is used to measure the distance at which two charged particles interact with each other. The coefficients $\kappa$ and $r_c$ are the inverse Debye
length and the cutoff radius applied to this interaction, respectively. The values $l_0 = 1.87$, $\alpha = 0.24$, $r_c = 3.00$, and $r_s = 0.10$ are used in the current study. In addition, similar to the modified conservative force, a maximum force, $F_{ij}^{\text{pulling}} = 100.00$ to the charged DPD particles within the distance of $r_i \leq 2r_s$ is introduced in our simulations.

The dynamics of polymer translocation are carried out by DPD simulations in the presence and absence of EIs. When the EIs are taken into account in the DPD simulations, the external applied driving force, $F_{\text{ext}}$, is considered to be an external applied electric force $F_{\text{ext}}^V$. When a charged DPD particle enters into the narrow pore, the external applied electric force may affect and drive it across the narrow pore. In the current study, the external applied electric force has the form, 

$$F_{\text{ext}}^V = -q_i V_{\text{ext}} z_i$$  \hspace{1cm} (9)$$

where $V_{\text{ext}}$ is an external applied voltage, $l_{\text{pore}}$ is the length of the narrow pore, and $z_i$ is a unit vector in the direction parallel to the narrow pore axis. On the other hand, if the EIs are absent in the DPD simulations, an external pulling force, $F_{\text{pulling}}$, which is equal to the electric force, $F_{\text{ext}}^V$, is still imposed on polymer monomers that reside in the narrow pore.

The simulations are performed using a modified version of the atomistic code named LAMMPS. Time integration of motion equations is calculated by a modified velocity-Verlet algorithm with $\lambda = 0.50$ and time step $\Delta t = 0.004$.

### 2.2. DPD Models

In the DPD approach, it is assumed that some molecules of the system are coarse-grained by a set of particles. Let us consider a homogeneous polymer chain with $N$ monomers (denoted by $P$). Each monomer has one effective negative unit charge $-q$. The valence $n$ of counter-ions is constrained to $+q$. Thus, the number of counter-ions is $N_c = qN/n$ with the electro-neutrality requirement in the simulated system. The simulation box is rectangular, with dimensions $L \times L \times 5L$ and $L$ varies in the simulations according to $N$. The narrow pore, as illustrated in Figure 1, is considered as a structureless cylindrical pore with length $l_{\text{pore}} = 2.00$ and diameter $d_{\text{pore}} = 1.75$. The wall of the narrow pore is formed by stationary DPD particles (denoted by W). We employ multi-layers of frozen DPD particles on the wall in combination with bounce-back reflections to prevent the penetration of polymer/solvent particles into the wall. For more details on the implementation of the wall boundary, we refer to ref. [54, 55].

Simulations for polymer molecules with chain lengths from $N = 25$ to 100 have been carried out under three different solvent conditions, i.e., good, $\theta$, and bad solvent conditions. One end of the polymer is initially placed and fixed at the entrance of the narrow pore, whereas the rest of the polymer monomers are placed randomly on the cis-side of the narrow pore. After the polymer is equilibrated, an external driving force is applied to the polymer monomers that reside in the narrow pore to drive them across it.

We monitor the instantaneous position of each polymer monomer during the translocation process. The translocation time is measured from the moment that the fixed end of polymer is pulled by the external driving force, to the moment that the entire polymer chain pass through the narrow pore. Once the fixed end of polymer molecule exits the cis-side of the narrow pore, the translocation event is failed. The translocation process is done when the polymer exits the narrow pore from the cis-side of it to the trans-side. We have performed our DPD simulations with totally independent initial conformations until at least 500 successful translocation events are obtained. The statistics over the successful translocation events are then evaluated, neglecting the failed runs.

### 2.3. Solvent Quality Model

Based on previous computational studies,[56,57] the repulsive parameters, $a_{ij}$, are adjusted to differentiate repulsions between unlike particles and like particles. Following Kong et al.,[49] the variation of repulsive parameter between polymer and solvent particles, $a_{PS}$, can be controlled by a solvent quality parameter, $\varepsilon$, which has the form

$$a_{PS} = a_{ij}(1 + \varepsilon)$$  \hspace{1cm} (10)$$
When \( \varepsilon < 0.00 \), repulsion between the polymer and solvent particles is weaker than that between two like particles, leading to preferential associations between these two particles (good solvent conditions). When \( \varepsilon > 0.00 \), repulsion between the polymer and solvent particles is strong, leading to preferential associations between two like particles (poor solvent conditions). Kong et al. showed that a parameter choice of \( \varepsilon < 0.00 \) leads to static scaling exponents \( v \) of 0.58–0.61 for the radius of gyration with polymer chain length.\(^{[49]}\) These values are consistent with the value \( v \approx 0.59 \), which characterizes the statistics of an excluded volume chain.\(^{[58]}\) They also found that \( v = 0.30–0.32 \) for \( \varepsilon > 0.10 \), which agrees with the theoretical value of \( v = 1/3 \) for a collapsed polymer chain. Analogously, Pan and Manke studied the effect of solvent quality on the dynamics of polymer solution via the DPD approach.\(^{[50]}\) In their simulations, they used \( \varepsilon = -0.30 \) to represent good solvent conditions and \( \varepsilon = 0.05 \) to represent poor solvent conditions. As suggested by Nardai and Zifferera,\(^{[51]}\) we expected that \( \varepsilon < 0.00 \) for good solvent conditions, \( \varepsilon \approx 0.09 \) for \( \theta \) solvent conditions, and \( \varepsilon \geq 0.20 \) for bad solvent conditions. Therefore, the solvent quality can be simply and accurately maintained by changing the repulsive interactions between the polymer and solvent particles.

According to previous computational studies,\(^{[51,56,59]}\) the repulsive parameter related to the interaction between two like DPD particles is \( a_{ii} = 25.00 \) (\( i = P, S, W \)), causing the simulated compressibility of these DPD particles at room temperature to correspond to the experimental value. In the simulations conducted in this study, we considered \( \varepsilon = -0.30, 0.09, \) and 0.30 to represent the good, \( \theta \), and bad solvent conditions, respectively; thus, the repulsive parameters were \( a_{PS} = 17.50, 27.20, \) and 32.50 for good, \( \theta \), and bad solvent conditions.

### 3. Results and Discussion

#### 3.1. Verification of the Electrostatic Interactions in DPD Simulations

We mainly considered the translocation of uncharged and charged polymers through a narrow pore under different solvent conditions. As suggested by Panwar and Muthukumar,\(^{[22]}\) the EIs of charged polymer monomers are represented by screened Coulombic interactions. It is technically difficult to present the EIs of charged particles with soft DPD interactions. As an effective simulation technique, DPD has been successfully applied in investigating a variety of soft matter problems for several years now because it can reproduce the correct hydrodynamic behavior of fluids. However, soft interparticle interactions also result in the overlapping among the DPD particles, which may give rise to strong ion pairing.

There have been some successful attempts to tackle this problem\(^{[60–62]}\); most proposed the replacement of the point charge at the center of the DPD particle with a charge distribution smeared across the particle. Groot developed a particle/particle–particle/mesh (PPPM) algorithm to spread out charges into the lattice.\(^{[60]}\) González-Melchor et al. included EIs into the DPD system through a modification in the Ewald sum method combined with charge distributions for DPD particles.\(^{[61]}\) These two methods were successfully applied to study charged polymers and polyelectrolyte surfactant solutions.\(^{[60,61,63]}\)

In our previous DPD simulations, we employed the PPPM method to study the conformational behaviors of charged/neutral star micelles in salt-free solution.\(^{[64]}\) In the current study, as suggested by Liu et al.,\(^{[53]}\) a rigid core was included in each DPD particle by modifying the form of the conservative force to avoid particle interpenetration problems based on the original DPD method. The overlapping and possible strong ion pairing of soft DPD particles in the original DPD model can be avoided to a large extent, because DPD particles with rigid cores can no longer penetrate each other. This gives us an alternative method through which we can take EIs into account simply by considering screened Coulombic interactions.

Several DPD simulation tests of charged polymer chains in aqueous solution were carried out to verify the accuracy of the EIs via screened Coulombic interactions. Figure 2 shows the curve of electrostatic forces for charged particles obtained from the DPD simulation. The analytical form of EIs shown in Equation 8 was then used as target with which to make direct comparisons. Figure 2 shows that the DPD simulation data (criss-crosses) quantitatively reproduced the curve from the analytical form of the electrostatic force. The agreement between these two electrostatic forces was good, so the EIs of the charged DPD particles can be simply represented through screened Coulombic interactions.

![Figure 2. Responses obtained through screened Coulombic interactions according to Equation 8 (solid lines) and statistical electrostatic forces at different distances between two charged DPD particles (criss-crosses) from the simulations.](attachment:image)
3.2. Polymer Translocation Without Considering Electrostatic Interactions

The translocation of polymers through the narrow pore was carried out under different solvent conditions and the dynamics of polymer translocation was described by its $\tau$. For comparison, we first calculated the average $\tau$ of a freely jointed polymer chain, in which the EIs were neglected in the simulations. Instead, an external pulling force, $F^{\text{pulling}}$, equal to the external applied electric force, $F^{*}$, was imposed on the polymer monomers that resided in the narrow pore. The effect of solvent quality on polymer translocation was then studied by changing the $a_{PS}$. As we stated earlier, an $a_{PS} = 17.50$ was imposed for good solvent conditions, $a_{PS} = 27.20$ for $\theta$ solvent conditions, and $a_{PS} = 32.50$ for bad solvent conditions. DPD simulations were carried out at these three $a_{PS}$.

Figure 3 shows the scaling relationships between the average $\tau$ and $N$ at these three different solvent conditions.

![Figure 3. Scaling of the average translocation time with respect to the polymer chain length, $\tau \approx N^\beta$, in the absence of electrostatic interaction. $\beta = 1.23 \pm 0.03$ (empty squares), $1.30 \pm 0.02$ (empty circles), and $1.39 \pm 0.04$ (empty triangles) in good, $\theta$, and bad solvent conditions, respectively.](image)

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Table 1. Summary of DPD simulation results. Here, $F$ is the driving force, $\beta$ the scaling exponent of the translocation time $\tau$ as a function of the polymer chain length $N$.

<table>
<thead>
<tr>
<th>Solvent condition (SC)</th>
<th>$F^{\text{pulling}}$ (without EIs)</th>
<th>$F^*$ (with EIs)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Good SC</td>
<td>$1.0$</td>
<td>$1.49 \pm 0.04^{a)}$</td>
</tr>
<tr>
<td></td>
<td>$10.0$</td>
<td>$1.23 \pm 0.03^{b)}$</td>
</tr>
<tr>
<td>Bad SC</td>
<td>$1.0$</td>
<td>$1.27 \pm 0.02^{c)}$</td>
</tr>
<tr>
<td></td>
<td>$10.0$</td>
<td>$0.98 \pm 0.03^{d)}$</td>
</tr>
</tbody>
</table>

$^{a)}$The scaling relationship is consistent with previous theoretical predictions$^{[30,31]}$ that $\tau \sim N^{1.49 \pm 0.04}$.

$^{b)}$The scaling relationship is consistent with previous theoretical predictions$^{[39,40,65]}$ that $\tau \sim N^{1.23 \pm 0.03}$.

$^{c)}$The scaling relationship is consistent with previous theoretical predictions$^{[38,44,66]}$ that $\tau \sim N^{1.27 \pm 0.02}$.

$^{d)}$The scaling relationship is consistent with previous theoretical predictions$^{[38,44,66]}$ that $\tau \sim N^{0.98 \pm 0.03}$.

3.3. Polymer Translocation Considering Electrostatic Interactions

Translocation of charged polymers through the narrow pore was carried out under an external applied electric force. In this case, each polymer monomer has an effective negative charge. When an external electric force is exerted on the charged polymer, the polymer can be drawn through...

![www.MaterialsViews.com](image)
The translocation of polymers through a narrow pore is a complex phenomenon involving competition between many-body particle/particle interactions and hydrodynamic coupling between the polymer and solvent particles, as well as interactions between the charged monomers and counter-ions. The EIs between charged monomers lead to the rich behavior of charged polymer solutions that is qualitatively different from that of uncharged polymer solutions. To understand the linear scaling relationships for the translocation of charged polymers under good and θ solvent conditions, the configurations of the charged monomers before entering the narrow pore and after exiting it during the translocation process should be considered. We now study the conformations of charged polymers to obtain a possible reason for the above results. To better understand chain configurations involved in the problem, we introduce the concept of an electrostatic blob. For a fully flexible polymer chain under good solvent conditions, the relation between blob size, r, and the number of monomers in it, g, is \( r \approx g^{3/5} \). The energy of the EIs among all charged monomers inside a blob is in the order of the thermal energy, \( k_B T \), thus,

\[
\frac{I_{bb}(fg)^{2/3}}{\xi} \approx \frac{l_0}{r_0} f^2 g^{7/5} \Rightarrow 1
\]

This leads to the following relation between the blob size and the fraction of charged monomers: \( \xi \approx r_0 (l_0/(l_b f))^3/7 \).

In the current study, the values \( l_0 = 1.87 \), \( r_0 = 0.60 \), and \( f = 1.00 \) (fully charged polymer) were used. Thus, the blob size was \( \xi \approx 0.37 \). Analogously, we obtained a blob size of \( \xi \approx r_0 (l_0/(l_b f))^{1/3} \approx 0.41 \) for a charged polymer within θ solvent conditions, which is more than twice the preset rigid core diameter of a charged monomer. EIs at a length scale \( r_c = 3.00 \) larger than the blob size lead to the elongation of the charged polymer chain into an array of blobs, which is qualitatively different from the swollen or coiled state for uncharged polymer chains before entering

**Figure 4.** Functional dependence of the probability of translocation of polymer through a narrow pore on external applied voltage obtained from simulations.

**Figure 5.** Scaling of the average translocation time with respect to the polymer chain length, \( \tau \approx N^3 \), in the presence of electrostatic interaction. \( \beta = 0.98 \pm 0.01 \) (empty squares), \( 1.04 \pm 0.01 \) (empty circles), and \( 1.29 \pm 0.02 \) (empty triangles) in good, θ, and bad solvent conditions, respectively.
the narrow pore and after exiting it during the translocation process. The configurations of charged polymers are extended during the whole translocation process; thus, a linear scaling relationship between the average \( t \) and \( N \) for good and \( \theta \) solvent conditions was obtained in the simulations. For an uncharged polymer chain under bad solvent conditions, there is an effective attraction between monomers, which causes the uncharged polymer chain to collapse into a dense spherical globule to minimize the number of unfavorable polymer/solvent contacts. Upon charging, the polymer globule changes its shape and size by splitting into a set of smaller charged globules (charged monomers connected by strings), thus yielding a smaller \( \beta \) for charged polymers than that for uncharged polymers in bad solvent conditions.

In a recent DPD simulation study on polymer translocation, Feng et al. obtained similar \( \beta \), which ranged from 0.94 to 0.98, by varying the dissipative radii. In their simulations, a long distance attractive interaction was included in the DPD particles, which was different from the soft DPD repulsive forces in the original DPD method. The modified Lennard-Jones force in their DPD simulations and the electrostatic force in our simulations may have a similar effect on the polymer molecules. From their results and ours, long distance interactions appear to play an important role in forced polymer translocation. Furthermore, as forced translocation is a highly non-equilibrium process, and the dynamics of translocation of polymers are strongly dependent on the method by which the external driving force is applied, the differences obtained from experiments, theories, and computer simulations are confirmed to exist, and differences in \( \beta \) for the translocation of polymers with and without EIs under different solvent conditions are reasonable.

In addition, according to previous studies, the HIs have also considerable influences on polymer translocation process. Experiments are carried out in three dimensions, and the effects of HIs must be taken into account if we are to understand their effect on forced polymer translocations. In order to better understand the role of HIs on the polymer translocation process, we present extensive simulations on the flow-induced translocation of polymers through a fluidic channel in the presence and absence of HIs.

According to Groot et al., one knows that the only difference between the DPD and Brownian dynamics method is that HIs are taken into account in the former method, but they are absent in the latter method. Thus, we can make a very pure comparison to see what happens if only HIs is turned off while all other physical effects are included. The scaling relation \( t \sim N^\beta \) is also obtained with \( \beta = 1.21 \pm 0.04 \) considering HIs and \( \beta = 1.37 \pm 0.03 \) without considering HIs for polymer translocation under good solvent conditions, which is in consistent with previous simulation results.

However, in a recent DPD simulation study on polymer translocation, Feng et al. observed the scaling exponent varied with the dissipative radii. In their simulations, a long distance attractive interaction was included in the DPD simulations, which was different from the soft DPD repulsive forces in the original DPD method. Thus, there might be some difference on the scaling exponent obtained from DPD with those from LD studies.

### 3.4. Waiting Time for Monomers

To further understand the behavior, we examine the dynamics of a single monomer passing through the narrow pore during translocation. The non-equilibrium nature of translocation has a significant effect on it. We have numerically calculated the waiting times for all monomers in a polymer chain. Here, the waiting time of monomer \( s \) is defined as the time duration between the events that monomer \( s \) and monomer \( s + 1 \) exit the narrow pore.

In Figure 6 we show the waiting time distribution for \( N = 100 \) under driving force \( F = 10.0 \) both with and without EIs. For polymer translocation without EIs, the monomers in the middle of the polymer need the longest time to translocate and the distribution is close to symmetric. Whereas for polymer translocation with EIs, the waiting time increases almost the whole translocation process, and the waiting time of monomers with \( s > 20 \) is larger than that without EIs. One of the possible reasons for the translocation of polymer in the presence of EIs is that the short distance repulsions among charged monomers slow down the translocations.

![Figure 6. Waiting time distribution for N=100 under driving force F=10.0 without and with electrostatic interactions. The waiting time of monomer s is defined as the time duration between the events that monomer s and monomer s+1 exit the narrow pore.](image-url)
that the scaling exponents depend significantly on the presence of EIs, respectively. These results demonstrate under good solvent conditions.

\[ \beta = 1.23 \pm 0.03 \] (empty squares) without electrostatic interactions and \( \beta = 0.98 \pm 0.03 \) (empty upwards pointing triangles) with electrostatic interactions. For \( F = 1.0 \), \( \beta = 1.49 \pm 0.04 \) (empty circles) and \( \beta = 1.27 \pm 0.02 \) (empty downwards pointing triangles) in the absence and presence of electrostatic interactions, respectively.

**3.5. Influence of the Driving Force**

Next we determine the average \( \tau \) as a function of driving force \( F \) under good solvent condition. For the scaling exponents \( \alpha \) defined as \( \tau \sim F^\alpha \), we obtain \( \alpha = -0.94 \pm 0.01 \) without considering EIs and \( \alpha = -0.99 \pm 0.01 \) with EIs, respectively, see Figure 7(a). Hence, the translocation time essential scales as \( \tau \approx F^{-\alpha} \), as is to be expected for the driving force values larger than the thermal fluctuations.\[45]

The average \( \tau \) scales with polymer length \( N \), both with and without EIs, is then measured at different driving forces under the same solvent conditions, see Figure 7(b). It is noteworthy that there exists no single scaling and \( \beta \) varies with the driving force. In the current study, the \( \beta \) increases with the decrease in \( F \). For strong driving forces, we obtain \( \beta = 1.23 \pm 0.03 \) at \( F_{\text{pulling}} = 10.0 \) without EIs and \( \beta = 0.98 \pm 0.03 \) at \( F^V = 10.0 \) with EIs. Decreasing \( F \) to 1.0, we obtain \( \beta = 1.49 \) and \( \beta = 1.27 \) in the absence and presence of EIs, respectively. These results demonstrate that the scaling exponents depend significantly on the driving force.

**4. Conclusion**

In this paper, we studied the effect of electrostatic interactions on the dynamics of translocation of polymers through a narrow pore under different solvent conditions via the particle-based dissipative particle dynamics (DPD) approach. The results showed that the average \( \tau \) versus \( N \) satisfied the scaling law \( \tau \approx N^\beta \). The \( \beta \) depended on the solvent quality, both in the presence and absence of electrostatic interactions. The \( \beta = 0.98 \) considering EIs and \( \beta = 1.23 \) without considering EIs for polymer translocation under good solvent conditions. \( \beta \) increased to 1.04 considering EIs, and to 1.30 without considering EIs under \( \theta \) solvent conditions. Under bad solvent conditions, the \( \beta \) further increased to 1.29 and 1.39 in the presence and absence EIs, respectively.

The scaling exponents are demonstrated to be significantly dependent on the driving force. For strong driving forces, we obtain \( \beta = 1.23 \) at \( F_{\text{pulling}} = 10.0 \) and \( \beta = 0.98 \) at \( F^V = 10.0 \) with EIs. Decreasing \( F \) to 1.0, we obtain \( \beta = 1.49 \) and \( \beta = 1.27 \) in the absence and presence of EIs, respectively. The findings in this work may help facilitate understanding of the dynamic behaviors of various polymer and/or DNA molecules during translocation processes.

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