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Research Article

A Semiflexible Polymer Translocation Through a Cylindrical Channel

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Abstract

In this study, translocation of a semi flexible polymer through a cylindrical channel have been investigated. A two-dimensional Monte Carlo simulation was employed, by utilizing the bond fluctuation method (BFM) to investigate the translocation processes of a chain length N. To surmount the entropic barrier, the middle monomers of the polymer have been positioned at the center of the pore, which is situated between the CIS and TRANS regions. Consequently, the static properties of a semi-flexible polymer by calculating the mean square end-to-end distance $\langle R^2\rangle$ and the mean square radius of gyration $\langle R_g^2\rangle$ as functions of the chain length (N) have been examined. The mean square end-to-end distance and the mean square radius of gyration are proportional to the number of monomers N as $\langle R^2\rangle \sim N^{1.496}$ and $\langle R^2 g\rangle \sim N^{1.505}$ correspondingly for a short cylindrical channel length L = 2, which aligns with the theoretically predicted. These finding indicates that the relationships between $\langle R^2\rangle$ and $\langle R_g^2\rangle$ and the polymer chain size N are strongly influenced by the channel length L. The dynamic properties by analyzing the translocation time of the polymers also studied. Additionally, the relationship between the escape time τ and the polymer chain length N depends on the pore width W, which is equivalent to the diameter of the cylindrical channel. These research demonstrates that the escape time τ decreases as the width increases and escape time τ increases as the chain stiffness increases.

Keywords

Semiflexible Polymer, Translocation, MC, BFM, Chain Stiffness

1. Introduction

Polymer have been of great interest in biology, chemistry, engineering and physics.

Semiflexible polymeric materials are crucial in numerous technological applications and serve as the foundation for many biological entities [1, 2, 6, 7, 8]. On the molecular scale, life itself is composed of biopolymers such as DNA, RNA, and proteins, which are essential to biological structures [3, 4, 10, 25]. Polymers are used specially, in optical, electronic, chemical, pharmaceutical and medical industries as main components of highly functional substance [5]. The functionality of polymer is because of their many advantages polymeric substance compered to metals, for instance, thermally and electrically insulating, radiolucency, low weight and lower process as well as lower maintenance cost [9, 11, 13-17]. The static properties of polymers are characterized by the size and shape of the polymer chain. Conversely, the dynamic properties of polymers are characterized by aspects such as the probability distribution of escape time and trans-

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location time as functions of chain length. The question of how a polymer chain moves in confined spaces has puzzled scientists for several decades. To answer this question, they study polymer translocation.

Polymer translocation is the process in which a polymer chain passes through a narrow channel or pore. This phenomenon is crucial in the fields of polymer physics and biophysics and plays a significant role in various biological processes, such as DNA replication and protein transport [10, 11, 22].

Translocation of semiflexible polymers through cylindrical channels has garnered significant interest due to its relevance in various biological and nanotechnological applications.

Additionally, translocation process plays a vital role in a various technological application like, rapid DNA sequencing, gene therapy and drug delivery [12, 18, 19, 23, 24]. A significant portion of theoretical and simulation research has focused on the translocation dynamics of fully flexible chains. However, many biopolymers, including dsDNA, proteins, actin, and microtubules, exist as semiflexible polymers [8, 9]. Therefore, it is essential to extend the study of polymer translocation to include semiflexible chains. Given their distinct behavior and broad applications, understanding biological phenomena necessitates modeling and simulations across different time and length scales to comprehend their static and dynamic properties, especially regarding the translocation of semiflexible polymers. The system was modeled by considering all particle interactions, which requires significant computational effort. The two well-known methods used to simulate polymers are molecular dynamics (MD) and the Monte Carlo (MC) method. however, Molecular dynamics (MD) method uses time average and Monte Carlo (MC) method uses ensemble average to simulate polymer. The difference between them lies in how they sample the configuration space available to the system. Basically, molecular dynamics simulates molecular movement by solving newton’s equation of motion for the molecule. Whereas, Monte Carlo method calculates thermodynamic statistical probabilities of acceptance or rejection of moves. To determine the parameters of static and dynamic properties of semi-flexible polymers using the Monte Carlo (MC) method, the bond fluctuation model (BFM) have been employed. This study investigates how the length of a cylindrical channel affects the static and dynamic properties of semi-flexible polymer translocation from the CIS side to the TRANS side in a 2D setup. Additionally, the impact of cylindrical channel length and chain stiffness on the scaling exponents of the mean square end-to-end distance $\langle R^2 \rangle$, mean square radius of gyration $\langle R_g^2 \rangle$, and the probability distribution of escape time (τ) as functions of the semi-flexible polymer chain length N have been analyzed. Furthermore, how the diameter of the cylindrical channel influences the translocation time (escape time) of semi-flexible polymers have explored. Finally, the effects of chain stiffness on the translocation time (escape time) in relation to the chain length N of semi-flexible polymers have been examined.

2. Methods and Model

Monte Carlo (MC) and Molecular Dynamics (MD) are widely recognized as the most popular techniques for simulating a wide range of systems and phenomena. Among these methods we used Monte Carlo (MC) simulation method [26, 28] due to the possibility of acceptance and rejection, conformation of a semi flexible polymer as stochastic process. In order to carrying out our simulation task, we required model. Therefore, used bond fluctuation model (BFM) to complete our simulation task.

2.1. Bond Fluctuation Method

The Bond Fluctuation Model (BFM) is a lattice model designed for simulating polymer systems, first introduced by Carmesin and Kremer in 1988 [24]. It is particularly useful for studying both static and dynamic properties of polymers. In this model, trial conformations are generated by moving a randomly selected monomer from its current position to a neighboring lattice site, chosen randomly and with equal probability among available directions.

During this move, it is crucial to prevent bond crossings and ensure the self-avoidance condition, where no monomer occupies the same lattice site simultaneously. The acceptance or rejection of these trial conformations follows the Metropolis algorithm, which determines whether a move improves the system's energy or conformal stability.

Implemented on a two-dimensional square lattice with a lattice constant of unity, each monomer can occupy any of the four neighboring lattice sites within a unit cell [27, 29]. Bonds between adjacent monomers in the polymer can only assume lengths of $2, \sqrt{5}, \sqrt{8}, 3, \sqrt{10}, \sqrt{13}$ lattice units [24]. The model focuses on a one-site representation for a semi-flexible linear polymer on the square lattice, ensuring that bond lengths remain between 2 and 4 lattice units to prevent bond crossings [30].

2.2. Simulation Procedure

In this computational study of semi flexible chain linear polymer, square lattice model have used by Monte Carlo simulation via bond fluctuation method. The goal is to explore both the static and dynamic properties of semi-flexible polymers. In the simulations, 2D square boxes measuring 500×500 lattice units utilized, with each unit representing a standard length. The positions of polymer monomers was monitored by capturing snapshots at regular intervals. The spacing between lattice points is sufficiently large to ensure it does not influence any properties of the polymer system significantly. Additionally, the excluded volume effect was enforced, ensuring that each lattice site can accommodate no more than one polymer monomer at a time. This condition mimics real-world constraints where polymers cannot occupy the same space simultaneously, influencing the overall configuration and behavior of the system. The bond length between neighbors will set as permitted by bond fluctuation method on $2D$ square lattice. In this simulation, the channel wall is constructed using a row of immobile monomers arranged in a straight line, spanning a length L in lattice units, which defines the channel's length. Both L (length) and W (width) of the channel are free parameters that significantly impact the dynamics of polymer translocation. Because of this, to investigate effects of channel length (L) and width (W) on dynamical properties of polymer translocation, they were fixed before starting the trial move. Channel length L=12 and channel width W = 6 was choose to construct cylindrical channel (pore) and the cylindrical channel (pore) is small enough to allow only one monomer or two monomers at minimum separation to pass through it as illustrated on figure 1.

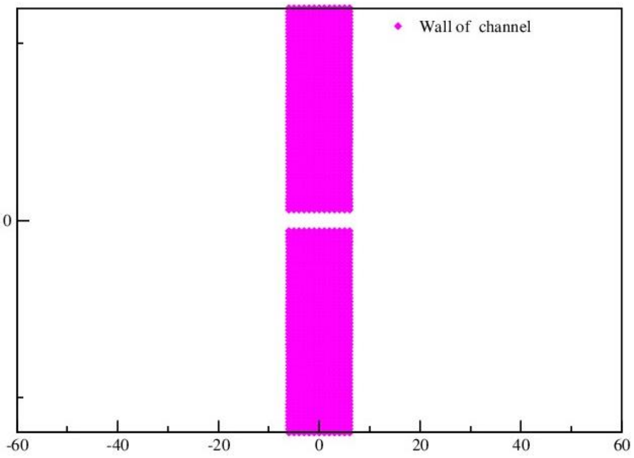

Figure 1. *A cylindrical channel of length L = 12 and width of W = 6 lattice units on the wall.*

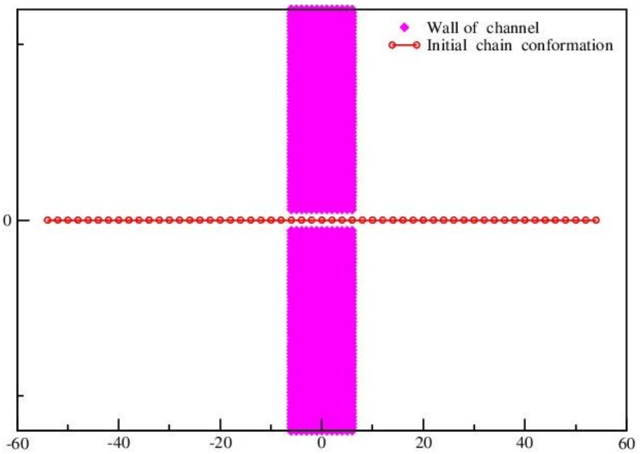

Figure 2. *The initial conformation of a linear polymer chain N = 55 that placed symmetrically in middle of channel at* $^{L}/_{2}$.

The linear polymer is initially positioned at the midpoint of the pore, spanning across both sides of the channel wall, with half of the chain on each side [31], as illustrated in Figure 2.

As shown on figure 2, the initial condition that shows how the polymer placed in the channel plays an important role in the determination of non-equilibrium process. In this setup, a polymer of size N is initially positioned such that the number of monomers n on each side of the pore is equal (i.e., left and right) from the center of the channel. This configuration is designed to ensure an equal probability of translocation to either side of the channel. Therefore, in this study, the polymer have placed symmetrically at the center of the pore initially to overcome the entropic barrier. Specifically, the initial configuration involves fixing the middle monomer $\frac{(N+1)}{2}$ at the midpoint of the channel. The remaining monomers are then equilibrated for a duration longer than the relaxation or equilibration time $\tau_{equil} \sim N^{2.5}$ for an unforced polymer in two dimensions. Starting from the initial polymer conformation, numerous moves were made until the polymer reached equilibrium. During this equilibration process, the polymer chain was allowed to relax through local moves. Each move involved randomly selecting a monomer and attempting a trial move by one lattice unit. The move was accepted if it did not violate the excluded volume constraint, maintain chain connectivity, and uphold the condition that the chain remains uncrossed. This iterative process continued until the polymer achieved a relaxed and equilibrated conformation. Furthermore, the metropolis algorithm test was followed if the chain had interaction energy J. After completing the equilibration process, at $t = 0$, the previously fixed middle monomer is allowed to move freely. The simulation continues until a time $t = t'$ >0 when the entire polymer has translocated to one side of the membrane, which was define as the escape time t' This procedure is repeated multiple times for each polymer length N, and the escape time τ that occurs most frequently across these simulations was record. This approach allows us to statistically analyze the translocation dynamics of the polymer under various conditions and lengths.

Numerically, τ can be sampled much more efficiently than τ_{tran}, where τ_{tran} is defined as the time that the polymer needs to translocate through a pore by putting the first monomer at the gate of the pore under a restriction that it never gets back, and the whole translocation process ends when the last monomer is on the other side of the pore. Numerically the escape time τ scales have been shown as $\tau^{1+2\nu}$ in agreement with our result [30]. This deliberate position is critical to overcome the impact of the entropic boundary or wall. The chain is then permitted to relax with neighborhood moves while one of its center monomer is fixed inside the pore as shown in Figure 3. After equilibration is finished, at t = 0, the middle monomer is allowed to move just like the rest of the monomers of the chain as shown in Figure 4.

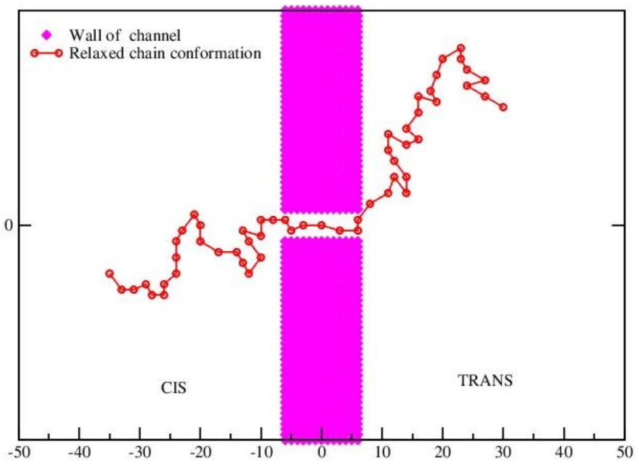

Figure 3. *Depicts a schematic of a linear polymer inside a cylindrical channel with a length L=12 units and width w = 6 units. The polymer chain shown has a length N = 55. This configuration represents the most likely state achieved after the polymer has undergone relaxation over N* × 10^6 *Monte Carlo moves.*

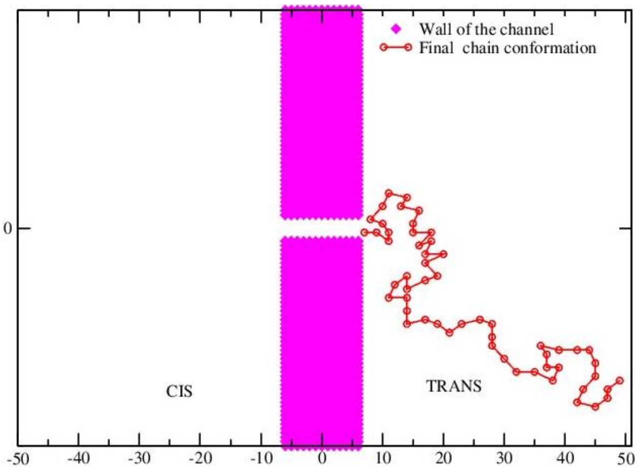

Figure 4. *After relaxing for N×10^6 Monte Carlo moves, a schematic representation shows a linear polymer of chain length N = 55 being translocated through a cylindrical pore with a length of L = 12 units and a width of W = 6 units.*

3. Results and Discussion

3.1. The Static Proper Ties of a Linear Polymer Chain

3.1.1. Mean Squared End to End Distance

The average conformation of a polymer can be determined by calculating the mean square end-to-end distance, which is a measure of the average distance covered by the polymer chain. This average distance is represented by the mean square end-to-end vector.

$$\langle R^2\rangle = \langle\overrightarrow{R_n^2}\rangle=\langle(\textstyle\sum_{i=1}^{n}\vec{r_i}).(\sum_{j=1}^{n}\vec{r_j})\rangle \tag{1}$$

The scalar product of two vectors, $\vec{r_i}.\vec{r_j}$, is given by their dot product. In this case, since all bond vectors have the same length, we can denote them as l. Therefore, the scalar product of the bond vectors is:

$$\vec{r_i}.\vec{r_j}=l \times l \times \cos\theta_{ij} \tag{2}$$

where, $\cos\theta_{ij}$ is the angle between $\vec{r_i}$ *and* $\vec{r_j}$ then, $\langle\cos\theta_{ij}\rangle$ = 0 for $i \neq j$ otherwise 1.

$$\langle\overrightarrow{R_n^2}\rangle=\textstyle\sum_{i=1}^{n}\ \sum_{j=1}^{n}\ \langle\ \cos\theta_{ij}\ \rangle \tag{3}$$

The mean square end-to-end distance is a static property of a polymer chain that depends on the number of monomers in the chain. In Figure 5, the plot of the mean square end-to-end distance $\langle R^2\rangle$ is shown as a function of the polymer chain length N, illustrating the interdependence of these parameters. In this study, the scaling exponent have been calculated by analyzing the slope of the log-log plot of $\langle R^2\rangle$ as a function of the number of monomers in the polymer, as depicted in Figure 5 for channel lengths L = 2, 4, and 12 units.

The log-log plot of $\langle R^2\rangle$ versus N for cylindrical channels with lengths L = 2 and 4 exhibits slopes of 1.496 and 1.475, respectively, which are consistent with Flory's prediction of the scaling exponent in two dimensions, as supported by previous works [20, 21, 33]. However, for a channel length of L = 12, the slope deviates slightly from Flory's prediction, measuring at 1.381.

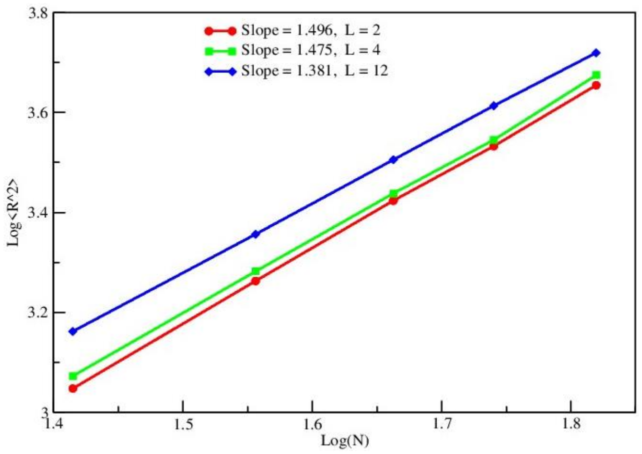

Figure 5. *The generated a log-log plot illustrating the mean square end-to-end distance* $\langle R^2\rangle$ *as a function of the polymer chain length N. The data points on the plot correspond to N values of 26, 36, 46, 55, and 66.*

3.1.2. The Calculation of the Mean-Squared Radius of Gyration

The mean square of the radius of gyration is often used as an alternative representation for the size of a polymer coil. It is defined as the average distance of a chain element from the center of gravity of the chain.

We have position vector $(\overrightarrow{R_{CM}})$ that expressed as;

$$\overrightarrow{R_{CM}} = \frac{1}{N}\sum_{j=1}^{n}\overrightarrow{R_J} \tag{4}$$

$$R_g^2 = \frac{1}{N}\sum_{j=1}^{n}(\overrightarrow{R_\iota} - \overrightarrow{R_{cm}})^2 \tag{5}$$

By expanding equation 5, we obtain:-

$$R_g^2 = \frac{1}{N}\sum_{j=1}^{n}(\overrightarrow{R_\iota}^2 - 2\overrightarrow{R_\iota R_{cm}} + \overrightarrow{R_{cm}}^2) \tag{6}$$

$$\langle R_g^2\rangle = \frac{\langle R^2\rangle}{6} \tag{7}$$

$$\text{Where, } \langle R^2\rangle = Nl^2 \tag{8}$$

The mean-square end-to-end distance $\langle R^2\rangle$ is related to the mean square radius of gyration $\langle R_g^2\rangle$ through the equation $\langle R^2\rangle = 6\langle R_g^2\rangle$. In Figure 6, the mean square radius of gyration $\langle R_g^2\rangle$ as a function of the polymer chain length N have been presented. The log-log plot of $\langle R_g^2\rangle$ versus N for channel lengths L = 2 and 4 exhibits slope of 1.505 and 1.481, respectively, which are in agreement with the Flory exponent as reported in previous works [20, 21, 33]. However, for a channel length of L = 12, a slope of 1.408 have been obtained, which is slightly closer to Flory's prediction.

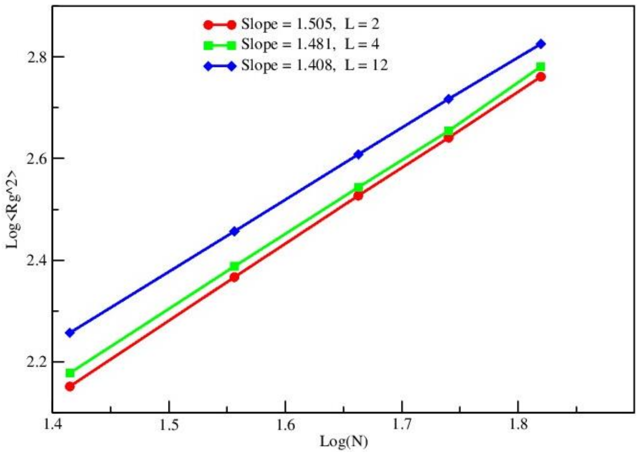

Figure 6*. The generated a log-log plot depicting the mean square radius of gyration $\langle R_g^2\rangle$ as a function of the polymer chain length N. The data points on the plot correspond to N values of 26, 36, 46, 55, and 66.*

The conformation of semiflexible polymers is also characterized by $\langle R^2\rangle$ and R_g^2 like as flexible chain polymer [11]. As described by Kaifu Luo et al. [32] the angle dependent bending potential that can describe flexibility, chain stiffness of polymer can be given by:-

$$\frac{U}{k_B T} = -\frac{J}{k_B T}\sum_{i=1}^{N-2}\cos\theta_i \tag{9}$$

where J *is* chain stiffness, N represents the number of monomers in the chain, θ_i represents the angle between two adjacent bonds, k_B is the Boltzmann constant, and T represents the absolute temperature.

In a linear polymer, the scaling of the equilibrium size can be described by the relation $\langle R^2\rangle \sim N^{2v}$, where N represents the number of monomers in the chain and v is a scaling factor. This scaling relationship provides valuable insights into the general scaling relation between the number of monomers and the radius of gyration of a polymer. Consequently, we can express this scaling argument as $\langle R_g^2\rangle \sim N^{2v}$. This scaling relation highlights the connection between the size of the polymer, characterized by the mean square radius of gyration $\langle R_g^2\rangle$, and the number of monomers N. It allows us to understand how changes in the polymer's length impact its overall size.

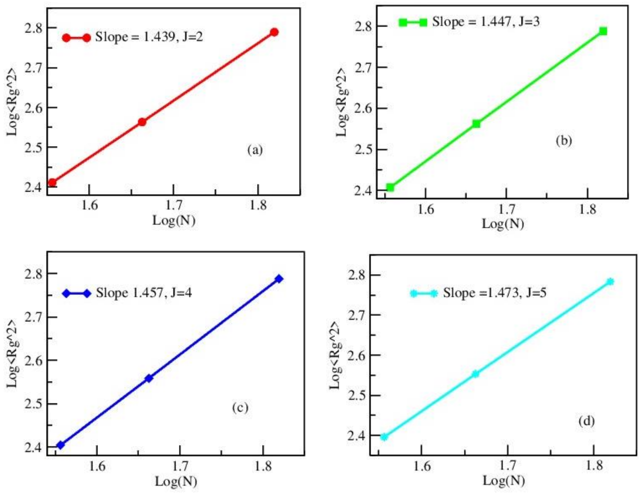

Figure 7*. The generated log-log plots depicting the mean square radius of gyration $\langle R_g^2\rangle$ as a function of chain length for specific values. For N = 36, 46, and 66, and chain stiffness values J = 2, 3, 4, and 5, the plots are represented as (a), (b), (c), and (d) respectively.*

In this computational simulation, the impact of chain stiffness on the scaling behavior of the mean square radius of gyration $\langle R_g^2\rangle$ have been investigated.

To achieve this, the interaction strength J have been varied and analyzed $\langle R_g^2\rangle$ as a function of chain length N, as demonstrated in Figure 7. This calculations have revealed the following scaling relationships: $\langle R_g^2\rangle \sim N^{1.349}$, $\langle R_g^2\rangle \sim N^{1.447}$, $\langle R_g^2\rangle \sim N^{1.457}$ and $\langle R_g^2\rangle \sim N^{1.473}$ for interaction strengths J = 2, 3, 4, and 5, respectively. The scaling exponents, determined as the slopes of the log-log plot of $\langle R_g^2\rangle$ as a function of chain length N, are found to be in agreement with the Flory exponent.

Remarkably, the examination has revealed that the chain stiffness, represented by the interaction strength J, does not affect the scaling exponent of $\langle R_g^2\rangle$ within the range of J values considered (J=0 to J=5). This finding aligns with the results reported in a related reference [35].

Through this comprehensive analysis, scaling behavior have been gained valuable insights into the relationship between chain stiffness and the mean square radius of gyration $\langle R_g^2 \rangle$. These findings contribute to understand polymer conformation and provide valuable information for future research endeavors.

3.2. Dynamic Proper Ties of a Semiflexible Linear Polymer

3.2.1. Probability Distribution of Escape Time

Figure 8 presents an intriguing observation regarding the probability distribution of the escape time of semiflexible linear polymers during translocation through a cylindrical channel. The plot showcases this distribution for chain lengths N = 16, 26, 36, and 66.

From the plot, it becomes evident that the simulation indicates that smaller polymers tend to escape in shorter times and have a higher probability of escaping compared to longer polymers within a given channel. This observation suggests that the size of the polymer plays a significant role in determining the translocation dynamics.

Understanding the escape time and probability distribution of polymers during translocation is crucial for various applications, such as drug delivery systems and nanopore sequencing technologies. These findings contribute to our understanding of the behavior of semiflexible linear polymers in confined environments and provide valuable insights for future research in this field.

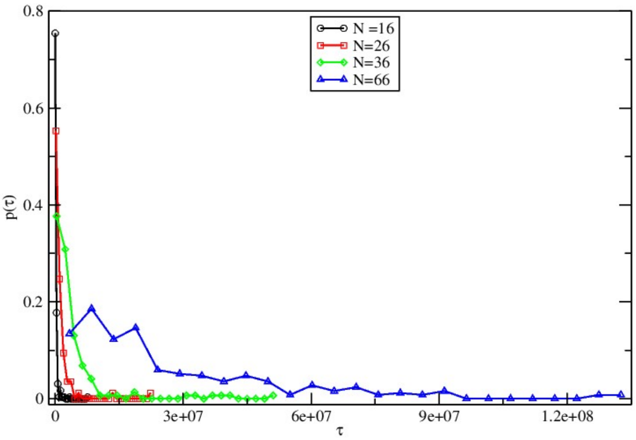

Figure 8. *The probability distribution P(τ) of the escape time τ for a linear polymer chain with different chain lengths N, specifically N = 16, 26, 36, and 66, was obtained through a total of 5000 simulation runs for each chain length.*

Figure 8 provides further insights into the behavior of the probability distribution P(τ) of the escape time for semiflexible linear polymers translocating through a cylindrical channel. As observed, the peak of P(τ) shifts towards higher values of τ as the chain length N increases. This shift can be attributed to the fact that larger N values require more time to escape from the channel.

Moreover, the probability distribution P(τ) exhibits a long-tailed distribution, indicating that it displays a sudden increase on the left side of the peak and an exponential decay on the right side. This characteristic is in contrast to a Gaussian distribution and reflects the skewed nature of the probability distribution, which is consistent with the findings reported in reference [36].

Understanding the shape and characteristics of the probability distribution P(τ) is crucial for gaining insights into the translocation dynamics of semiflexible linear polymers. These findings provide valuable information for characterizing and modeling the escape time behavior in confined environments.

3.2.2. The Relationship Between Translocation Time and Chain Length (N)

The analysis of the escape time τ in relation to the chain length for the translocation of semiflexible linear polymers have been conducted. To simulate the escape time τ as a function of chain length (N), a cylinder channel with dimensions L = 4 and a width of w = 6 lattice units have been utilized. The polymer chain lengths N = 26, 36, 46, and 66 have been considered, performing several thousand simulation runs for each case.

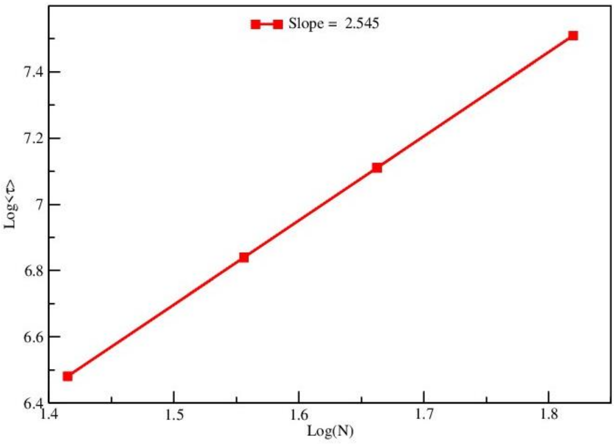

Figure 9. *The log-log plot showcasing the relationship between the escape time τ and the chain length N for a stiff polymer with chain lengths N = 26, 36, 46, and 66.*

From the obtained probability distribution, the most probable escape time have been determined and plotted it as a function of polymer chain length (N), as depicted in figure 9. By examining the log-log plot of the escape time τ against the polymer chain length (N), τ have been observed that $\tau \sim N^{\alpha}$, where α is given by $\alpha = 1 + 2v$. These simulation yielded a value of α = 2.545, which is in agreement with the expected value of

$1 + 2v$. The slight difference can be attributed to the presence of bending rigidity or chain stiffness.

In our simulation, $k_B T = 1$ and $J = 5$, indicating that the stiffness of the polymer does not impact the scaling behavior of τ. This finding aligns with the mathematical description of chain stiffness provided by equation 9.

Overall, the analysis of the escape time τ as a function of chain length (N) provides insight into the scaling behavior of translocation in semiflexible linear polymers. The agreement between the simulation results and the expected values further validates our findings.

3.2.3. Investigating the Impact of Channel Width on Translocation Time in Semiflexible Linear Polymers

In this extensive study, to investigate the impact of channel width have been endeavored, specifically the diameter of a cylindrical channel, on the average escape time of semiflexible linear polymers. In each simulation run, the most probable values of the escape time have been considered.

Furthermore, the relationship between the average mean escape time and the width of the channel have been examined. As depicted in figure 10, the simulation results revealed a noteworthy observation: the translocation time tends to decrease as the size of the pore, or channel width, increases. This finding indicates that when the size of the aperture enlarges, the resistance experienced by the monomers during translocation diminishes. This behavior aligns with the findings reported in reference [37].

By exploring the effect of channel width on the translocation time, the study contributes to a deeper understanding of the dynamics and behavior of semiflexible linear polymers in confined environments. These findings have implications for various applications, including nanopore-based technologies and drug delivery systems.

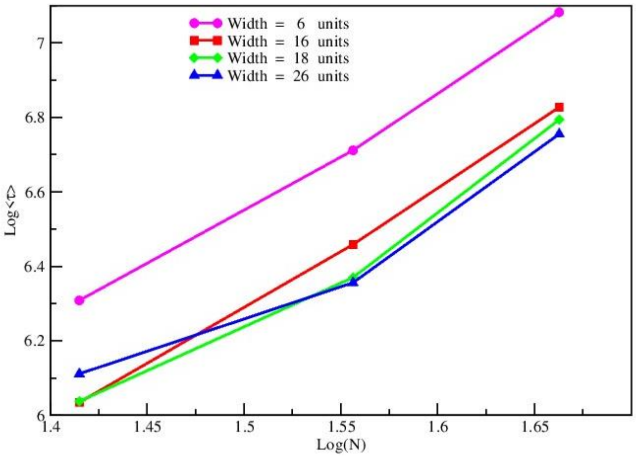

Figure 10. *Scaling behavior of escape time τ as a function of chain length N for N = 26, 36, and 46.*

3.2.4. Effects of Chain Stiffness on Mean Square Escape Time

In these computational simulation study, the influence of chain stiffness on the average translocation time of a given polymer have been delved. To explore the impact of chain stiffness, the interaction energy J have been varied, which corresponds to the bending constant or bending rigidity of the polymer.

Figure 11 presents the most probable translocation time as a function of the chain length for different values of J, specifically J = 0, 1, 2, 3, and 4. The results demonstrate that as the chain stiffness increases, the translocation time also increases. This finding aligns with the findings reported in relevant references [34, 38].

By examining the relationship between chain stiffness and translocation time, the study sheds light on the intricate dynamics of polymers and their behavior in confined environments. These insights contribute to a better understanding of polymer translocation and have implications for various fields, including biophysics and materials science.

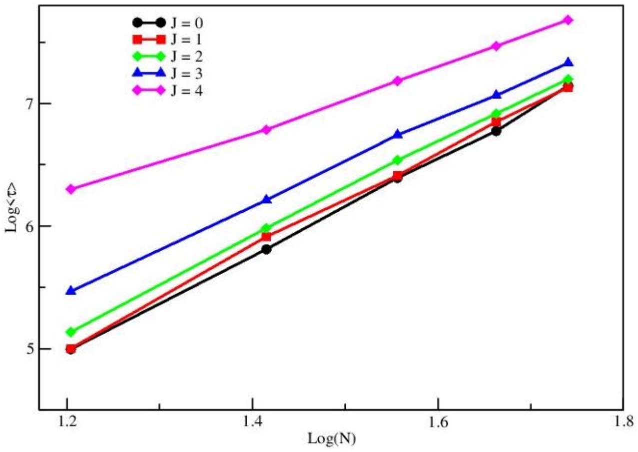

Figure 11. *The log-log plot illustrates the relationship between the escape time τ and the chain length N for the specified chain lengths N = 16, 26, 36, 46, and 55.*

Generally, as shown in figure 12, if the polymer chain has a larger stiffness, it tends to take a longer time to translocate compared to a chain with smaller stiffness.

The reason behind this is that a stiffer polymer chain has a higher resistance to bending and folding, making it more difficult for the chain to navigate through narrow pores or channels during translocation. On the other hand, a chain with smaller stiffness can more easily adopt conformations that allow it to pass through the pores or channels, resulting in a shorter escape time which is consistence with reference [34].

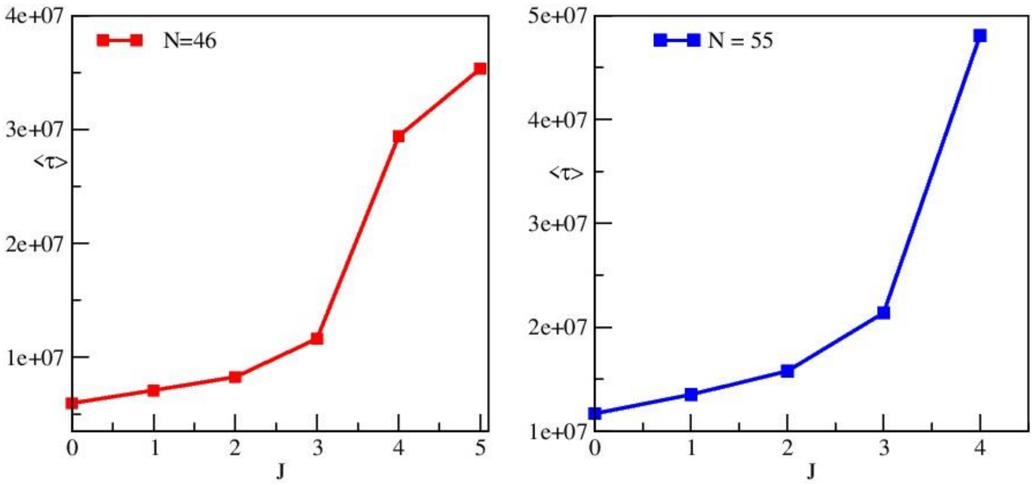

Figure 12. *The figure demonstrates the relationship between the mean escape time τ and the chain stiffness J for chain lengths N = 46 and N = 55.*

4. Conclusion

In these research, Monte Carlo simulations using basic lattice models to study semiflexible linear polymer chains with varying degrees of stiffness as they move through a cylindrical channel have been conducted. The numerical problem of polymer translocation through a cylindrical channel, focusing on the impact of chain stiffness have been explored. This investigation was based on the 2D fluctuating bond model, examining both the static and dynamic properties of the semiflexible linear polymer. The static properties were characterized by the end-to-end distance and the radius of gyration of the polymer chain.

The mean square end-to-end distance and the mean square radius of gyration are proportional to the number of monomers N as $\langle R^2 \rangle \sim N^{1.496}$ and $\langle R_g^2 \rangle \sim N^{1.505}$ respectively for short channel length (pore). Thus, the Flory law is satisfied in both scenarios for short channel lengths of the linear chain polymer. Additionally, how chain stiffness affects the static properties of semiflexible polymers have been examined, specifically the mean square radius of gyration. By increasing the chain stiffness J, this results indicated that chain stiffness does not influence R_g^2. The dynamic properties of a polymer chain, including the probability distribution of the polymer also explored, the scaling law of escape time as a function of chain length N, the effects of channel width on escape time, and the impact of chain stiffness on escape time. These finding indicates that the translocation time of a polymer chain is highly dependent on its length. The translocation time depends on the chain length as $\tau \sim N^{2.545}$ which aligns with the theoretically predicted value of $\tau \sim N^{2.5}$. The effects of channel width and chain stiffness on translocation time also analyzed. These results show that as the width of the channel increases, the escape time decreases, and as the chain stiffness increases, the escape time also increases.

Abbreviations

DNA	Deoxyribonucleic Acid
RNA	Ribonucleic Acid
EV	Excluded Volume
MC	Monte Carlo
MD	Molecular Dynamics
SAW	Self Avoiding Walk
BFM	Bond Fluctuating Method
R	End-to-End Distance
Rg	Radius of Gyration
kB	Boltzmann Constant

Author Contributions

Adugna Terecha Furi: Conceptualization, Data curation, Formal, Analysis, Funding acquisition, Investigation, Methodology, Resources, Software, Visualization, Writing – original draft, Writing – review & editing

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Data Availability Statement

The data is available from the corresponding author upon reasonable request.

Conflicts of Interest

The authors declare no conflicts of interest.

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