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# Investigation of Magneto Hydro-Dynamics Effects on a Polymer Chain Transfer in Micro-Channel Using Dissipative Particle Dynamics Method

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**Abstract:** In this paper, the effect of Magneto Hydro-Dynamics (MHD) on a polymer chain in the micro channel is studied by employing the Dissipative Particle Dynamics simulation (DPD) method. First, in a simple symmetric micro-channel, the results are evaluated and validated for different values of Hartmann (*Ha*) Number. The difference between the simulation and analytical solution is below 10%. Then, two types of polymer chain including short and long polymer chain are examined in the channel and the effective parameters such as *Ha* number, the harmony bond coefficient or spring constant (*K*), and the length of the polymer chain (*N*) are studied in the MHD flow. It is shown that by increasing harmony bond constant to 10 times with Ha = 20, the reduction of about 80% in radius of gyration squared, and half in polymer length compared to Ha = 1 would occur for both test cases. For short and long length of polymer, proper transfer of a polymer chain through MHD particles flow is observed with less perturbations (80%) and faster polymer transfer in the symmetric micro-channel.

**Keywords:** magneto hydro-dynamics (MHD); dissipative particle dynamics (DPD); Hartmann number (*Ha*-value); harmony bond coefficient or spring constant (*K*)

# 1. Introduction

Understanding the behavior of polymer chains in micro/nano-scale flows is an important issue, as it is the gateway to different scientific and technological research activities in different fields of study such as biology, genetics, etc. The translocation of polymers through nano/micro-scale passages is encountered in many biological processes in living cells or chemical processes such as DNA (Deoxyribonucleic acid) motion through narrow pores, protein translocation through cell membranes, and penetration of viruses into the cell nucleus. Knowledge of such processes can be beneficial in developing some technical analysis procedures concerning genomic partitioning and rapid DNA sequencing [1–3]. There are several ways to transfer polymer through narrow pores or micro channel including electroosmotic micro pump, magneto hydrodynamic method, and pressure driven flow [3]. Due to high controllability on fluid flow using electrical field or magnetic field, they are proper methods for fluid pumping [3,4].

The difficulties and costs associated with the experimental studies promote the researchers to use the computational simulation methods as the preliminary design and analysis tools to narrow down the design parameters' envelopes before getting into the actual manufacturing process. Regarding the small scale of simulated systems, molecular simulation methods would be the best choices. Such simulation methods have been successfully applied to different nano-scale flow problems. Researches have used different numerical simulation methods such as computational fluid dynamics [5–7], molecular dynamics [8], Langevin dynamics [9,10], and Brownian dynamics [11] to study prediction of polymer chains behavior in fluid flows. Based on the Lagrangian methods such as Molecular Dynamics [12–15], lattice Boltzmann method [16,17] or smoothed particle hydrodynamics method [18–21], the dissipative particle dynamics (DPD) method is a mesoscopic method [12,13,22] which has been vastly used in micro/nano-scale simulations. It benefits from the lower computational cost compared with the molecular dynamics method via using the clusters of molecules, known as beads, instead of considering all actual molecules.

There are several studies in relation of DPD and polymer chain motion in nano/micro flows. Zhang and Manke [23] used the DPD method to study the motion of polymers and polymer solutions rheology in the spherical particles with adsorbed polymers. They found that Newtonian behavior is governing on polymer solutions or polymer in sphere suspensions at low shear rates, but shear-thinning behavior is formed at higher shear rates. Willemsen et al. [24] used the DPD method to investigate the motion of a polymer within a square capillary and the effect of polymers on melting process in a shear flow. Pastorino et al. [25] compared the dynamics of Langevin and DPD as a thermostat term in non-equilibrium simulations of polymeric systems. They studied polymer brushes in different systems including the relative sliding motion, Poiseuille and Couette flows of polymeric liquids, and brush-melt interfaces to compare these two different thermostats. Based on the DPD method, Duong-Hong et al. [26] introduced an electrophoresis model for DNA, which they simulated the coupled DNA electro-osmotic and electrophoretic motion in micro/nano-scale passages. Using this model, they were able to capture the free-draining mobility of DNA while avoiding the expensive electrostatic interactions in the molecular simulations. They also computed DNA mobilities in realistic geometries with a good accuracy. Their results indicated that the Ti-channel has a better separating performance than the Tp-channel. Pan et al. [27] used the DPD method to study the DNA separation in a micro-device using an entropic trapping mechanism. They showed that longer DNA strands have a higher speed than shorter ones. They concluded that the entropic trapping is the consequence of delayed entrance. Moreover, they concluded that corner trapping does not contribute to DNA separation. Masoud and Alexeev [28] used the DPD method to design nano-structured surfaces capable of selective regulation of collision between microchannel walls and polymer, which is suspended in fluid though the microchannel. By utilizing different geometries for nanoscopic posts attached to the internal channel surfaces, they could attract the suspended nanoparticles and polymeric chains to the walls or repel them. Guo et al. [29] studied the translocation of polymers in fluid through a microchannel using the DPD method. They predicted the relation between shear stress and length of polymer chain for the average translocation time. Moreover, they observed two different mechanisms for translocation including single-file and double-folded translocation. They also mentioned the possibility of clogging at the entrance of the channel for polymers longer than a critical length.

All of the mentioned studies used pressure driven flow for transfer of polymer through microchannel. However, lack of studies in the area of different body forces are observed. Yang et al. [30] studied the motion of a polymer chain through a hole using DPD method. They considered two different driving forces, namely the uniform hydrostatic force implemented to whole solvent particles and polymer chains, and also uniform electrostatic force which is employed as a body force, applied to selected charged particles in the chain and some ions in the solvent which were charged oppositely. They found that the power-law correlations should be used for coil-like chains and it is not proper for globular chains. Ranjith et al. [31] used the DPD method to investigate the effect of finite slip at hydrophobic microchannel walls on the hydrodynamics and the dynamics of the DNA chain. They showed that an asymmetric velocity profile caused by hydrophobic and hydrophilic walls can affect the location of the DNA molecules. They used this effect to propose a simple arrangement for separation of short and long DNA chains. Zakeri [32] used the DPD method to simulate the performance of a soft polymer micro-actuator in electro-osmotic flow in a simple micro-channel and a convergent–divergent one. The results indicated that the amplitude of reciprocating motion of

polymer increases as the electric field is enhanced, the number of beads is decreased, the spring constant is increased, or more length of a polymer chain is exposed against the fluid flow motion.

A thorough review on the literature shows that there were studies in which the electrical field is used as the transport driving force for polymer chains, e.g., [26,32,33]. Base on the Zakeri [32,34], electroosmotic is a proper external force to move DPD particles in a micro channel, However, the transport of polymer chains using the magnetic forces is not regarded frequently. Magnetic force [35,36] is also another body force capable of inducing fluid flow. This driving force plays an important role in micro pumps (e.g., see [37–42]). Kefayati [43] employed LBM method to simulate the effect of MHD flow in a lid-driven cavity problem for various Hartman numbers. Ghahderijani [44] used LBM method to simulate MHD flow in simple micro channels. Javaherdeh and Najjarnezami [45] used LBM to investigate natural convection in a porous cavity with sinusoidally heated walls considering the effects of magnetic field. They investigated the effects of Hartmann number, porosity and Darcy number on the fluid flow, and heat transfer. Chaabane and Jemni [46] used the LBM to study the convection heat transfer in a 2D enclosure containing a conductive fluid. They examined the effects of Hartmann number, Rayleigh number, Prandtl number on the flow, and temperature fields. Although LBM is a proper simulation method in microscale, the freedom degree of DPD method is higher and it treats more realistically based on the real physics of particles interaction [17,47]. Based on the several references [32,34], the effect of polymer chain from electroosmotic flow was presented, but polymer transfer from in MHD flow requires more investigation.

In this paper, the DPD simulation method is employed to simulate MHD flow in simple symmetric micro channel, also the motion of a polymer chain through micro channel is studied to investigate the various physical properties of polymer chain influenced from MHD flow.

# 2. Numerical Simulation

To present the simulation of MHD in micro channels which affects the polymer chain transfer through fluid particles, we discuss in the three main subjects in the Sections 2.1–2.3, including the magneto-hydrodynamics equations, the details of DPD method, and the molecular model of polymer chain.

#### 2.1. Magneto-Hydrodynamics

Magneto-Hydro-Dynamics (MHD) equations consist of equations of electromagnetics and hydrodynamics. Electromagnetics equation relates the current density *J* to the magnetic field strength H [48–50].

$$curl \vec{H} = \vec{J} \tag{1}$$

$$div J = 0 \tag{2}$$

In the case that the substance such as fluid has a velocity, J is calculated as follows:

$$\vec{J} = \sigma(\vec{E} + \vec{v} \times \mu \vec{H})$$
(3)

where  $\sigma$  is the electrical conductivity, v is the velocity of flow,  $\mu$  is the magnetic permeability, and E is the electric field intensity. The body force or external force  $\vec{F}_e$  which will be used in DPD equations, Section 2.2 (as hydrodynamic equations) is calculated as follows:

$$\vec{F}_e = \vec{J} \times \mu \vec{H} \tag{4}$$

#### 2.1.1. Analytical Solution for MHD in Simple Channel

By using the source term  $F_{ex}$  calculated in Equation (4) in the steady equation of fluid motion, applying the assumption of uniform conductivity of liquid between two parallel walls (simple channel),

implementing  $H_0$  perpendicular to the walls in *z*-direction while implementing *E* in *y*-direction, and ignoring the gravity effect, a fluid motion should occur in *x*-direction satisfying the following momentum equation [47,51].

$$0 = \frac{-\partial p}{\partial x} + \mu J_y H_0 + \eta \frac{\partial^2 v}{\partial z^2}$$
(5)

where *p* is pressure term,  $\eta$  is the dynamic viscosity, and  $J_y = \sigma(E - v\mu H_0)$ .

Substituting the  $J_y$  in Equation (5) and assuming that velocity is zero at the walls and shear stress is zero at the middle of channel, would result in the following solution of MHD flow in the simple channel.

$$v = V_v \left(1 - \frac{\cosh\left(\frac{Ha}{L}z\right)}{\cosh\left(Ha\right)}\right) \tag{6}$$

where,  $V_v = \left(\frac{E}{\mu H_0} + \frac{\frac{-\partial p}{\partial x}}{\sigma \mu^2 H_0^2}\right)$  and  $Ha = \mu H_0 L \left(\frac{\sigma}{\mu}\right)^{0.5}$ . If the parameter  $H_0$  varies while the other parameters are kept constant, the value of Ha

If the parameter  $H_0$  varies while the other parameters are kept constant, the value of Ha (or Hartmann number) will change linearly. Hartmann number or Ha is the ratio of magnetic force to viscous force.

If we assume that 
$$V_v = 1$$
 then  $E = (1 - \frac{\frac{-\partial p}{\partial x}}{\sigma \mu^2 H_0^2})\mu H_0$  and  $J_y = \sigma((1 - \frac{\frac{-\partial p}{\partial x}}{\sigma \mu^2 H_0^2})\mu H_0 - \mu v H_0)$ 

### 2.2. Dissipative Particle Dynamics Method

The DPD method treats the simulated system as a cloud of beads each having the mass,  $m_i$ , position vector  $\vec{r}_i$ , and velocity vector  $\vec{v}_i$ . The evolution of beads' velocity vectors follows the basic kinematic and dynamic laws of motion [47].

$$\vec{v}_i = \frac{d\vec{r}_i}{dt} \tag{7}$$

$$m_i \frac{d\vec{v}_i}{dt} = \vec{F}_i \tag{8}$$

The net force exerted on bead *i* and  $\vec{F}_i$ , can be decomposed in two parts, namely the force exerted by an external force-field  $\vec{F}_e$  like gravitational, electrical, or magnetic fields, and the intermolecular forces exerted by polymer  $\vec{F}_{p,i}$  and fluid particles  $\sum_{j \neq i} \vec{f}_{ij}$ :

$$\vec{F}_i = \vec{F}_{p,i} + \sum_{j \neq i} \vec{f}_{ij} + \vec{F}_e$$
(9)

In DPD method, it is assumed that the intermolecular force exerted by bead j on bead i and  $f_{ij'}$  consists of three parts, namely the conservative force, the dissipative force, and the random force [52].

$$\vec{f}_{ij} = \vec{f}_{ij} + \vec{f}_{ij} + \vec{f}_{ij}$$
(10)

Of course,  $\vec{f}_{ij}$  would be equal to , as the third law of motion indicates.  $\vec{F}_{ext}$  is the external force such a electro-osmotic force or magnetic force [32].

The conservative force can be described using the following force filed:

$$\vec{f}_{ij}^{C} = \begin{cases} a_{ij}(1 - r_{ij}/r_{c})\hat{r}_{ij} & r_{ij} < r_{c} \\ 0 & r_{ij} \ge r_{c} \end{cases}$$
(11)

where  $a_{ij}$  is the maximum repulsion force between beads *i* and *j*,  $r_{ij}$  is the distance between those beads, i.e.,  $r_{ij} = |\vec{r}_{ij}|$ , and  $\hat{r}_{ij} = \vec{r}_{ij}/|\vec{r}_{ij}|$  is the unit vector pointing from bead *j* to bead *i*, and  $r_c$  is the cut-off radius beyond which, the intermolecular forces are assumed to diminish effectively.

The dissipative intermolecular force is calculated as follows:

$$\vec{f}_{ij}^{\rm D} = -\gamma \omega^{\rm D} r_{ij}(\hat{r}_{ij}.\vec{v}_{ij})\hat{r}_{ij}$$
(12)

where  $\gamma$  is a constant that determines the strength of dissipative force. The weighting function  $\omega^{D}$  is calculated as follows:

$$\omega^{\rm D}(r_{ij}) = \begin{cases} (1 - r_{ij}/r_{\rm c})^2 & r < r_{ij} \\ 0 & r \ge r_{ij} \end{cases}$$
(13)

On the other hand, the random force is calculated as follows:

$$\stackrel{\rightarrow \mathbf{R}}{f}_{ij} = -\sigma^{\mathbf{R}}\omega^{\mathbf{R}} r_{ij}\theta_{ij}\hat{r}_{ij} \tag{14}$$

in which, the constant  $\sigma^R$  determines the strength of random force.  $\vec{v}_{ij}$  is the relative velocity vector between beads *i* and *j*.  $\theta_{ij}$  is a random number chosen from a symmetric Gaussian distribution having the zero mean and unit variance.  $\sigma^R$  and  $\omega^R$  relate to  $\gamma$  and  $\omega^D$  as follows:

$$\omega^{\rm R} = \sqrt{\omega^{\rm D}} \tag{15}$$

$$\sigma^R = \sqrt{2\gamma k_{\rm B}T} \tag{16}$$

where  $k_{\rm B}$  is the Boltzmann constant and *T* is the temperature.

In this study, the modified velocity-Verlet algorithm is used for time integration of position and velocity of each particle is calculated explicitly. The Ref. [53] is suggested for more information. Implementation of wall boundary condition has been follow based on the ref [48,54–56].

#### 2.3. Polymer Chain

Polymer chain model consists of a number of masses and springs which are connected together. The mechanism of polymer chain motion influenced from interaction of fluid particles and polymer beads is depicted in Figure 1. According to number of different types of particles, we have different interactions. In this case, we have three types of interactions, including fluid to fluid particles, polymer and fluid, and polymer and polymer beads interactions. Each mass has its own repulsion force to fluid particles or other masses. Thus, the conservative force  $F_c$  should be modified for this type of simulation. In this paper, the harmonic spring force,  $\vec{f}_{i,i\pm 1}$ , or  $\vec{F}_{p,i}$  is used between beads which is added to  $F_c$  in DPD formulation. For the beads consisting a polymer chain, the following conservative harmonic force presents the intermolecular bonds [32,34,53].

$$\vec{f}_{i,i\pm 1}^{S} = -K(r_{i,i\pm 1} - r_{i,i\pm 1}^{eq})\hat{r}_{i,i\pm 1} = \vec{F}_{p,i}$$
(17)

where  $r_{i,i\pm 1}^{eq}$  is the equilibrium (zero-force) distance between two beads in the polymer chain and *K* is the harmonic bond constant.



Figure 1. Mechanism of polymer and fluid particles interaction and motion of polymer chain.

Due to difficulty of studying the properties of polymer chain in motion, some physical properties such as mean square radius of gyration and velocity of mass center are employed for finding effect of MHD on polymer chain motion.

In equilibrium, the radius of gyration is defined as [30,51]:

$$\langle R_G^2 \rangle = \frac{1}{2N^2} \langle r_{ij}^2 \rangle \tag{18}$$

where,  $r_{ij} = |\vec{r}_i - \vec{r}_j|$  and *N* is the number of beads of polymer chain. The end to end distance (Ee) is defined as  $\langle R_G^2 \rangle = \langle r_{N1}^2 \rangle$ . Also, the center of mass velocity of system is calculated as follows:

$$v_{\rm cm} = \frac{\sum_1^N m_i v_i}{\sum_1^N m_i} \tag{19}$$

where  $m_i$  is the mass of bead *i*. Also, the average kinetic temperature is calculated as follows [51].

$$\langle k_B T \rangle = \frac{m}{3n-3} \langle \sum_{1}^{n} v_i^2 \rangle \tag{20}$$

where *n* is the number of particles.

# 3. Results

In this section, the results of numerical simulations of MHD flow in micro channel are presented regarding the polymer chain motion under the influence of magnetic field (MHD flow) using DPD method. We developed our DPD code for current simulation. First, the DPD results for the simple channel flow with the results of the analytical solution are compared to evaluate the accuracy of suggested method for this type of simulation. Then, the study by embedding the polymer chain in a simple channel is extended to study the effect of MHD flow on polymer chain and the related motion characteristics. Different conditions have been considered including changing the magnetic field or *Ha*-value, spring constant (harmonic bond constant of polymer), or *K* parameter and the number of polymer beads in the polymer chain.

# 3.1. Validation of MHD-DPD Results with Analytical Solution

In order to evaluate and validate the results, the simple microchannel flow under external force of magnetic field is simulated. The simulation parameters are presented in Tables 1–3. The analytical velocity profiles are also calculated in accordance with Equation (6) in Section 2.1.1 with the assumption of  $V_v = 1$ . As can be seen in Figure 2 (left), by increasing the value of parameter Ha Number,

dimensionless velocity profiles not only increase to a certain extent in terms of value, but they also flatten more in plug like shape and tend to remain constant thereafter. For example, there is a dramatic change of about 80% for maximum value of dimensionless velocity when the value Ha Number is increased from 1.0 to 2.0. However, the changes are much less evident from Ha = 10 to Ha = 20. For a better study of variation of MHD flow, the dimensionless average velocity of particles in channel considering different values of Ha is compared with the analytical calculation in Figure 2 (right). As it is expected, increasing the value of Ha, the differences would decrease remarkably and would approach the constant value of unity. Also, the results show a proper agreement with the analytical results. The range of discrepancy between DPD solution and analytical solution is between 3% to 7%. The level of accuracy depends on time steps and number of iterations. Therefore, the parameter of Ha number is a suitable criterion for studying the velocity profile behavior in micro-channels and DPD method is a proper method for this type of fluid simulation.

Table 1.	Setting	parameters	for	particles	of DPD.
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Variables	$a_{ij}$ Different Particles	<i>a<sub>jj</sub></i> Same Particles	Number of Particles	Simulation Box (Channel Size)	Time Step	σ	γ	Cut Off Radious	Periodic Boundary Condition
Value	3	10	4000	20 (length) $\times$ 50 (height)	0.001	3	4.5	1	x-direction

Table 2. Setting parameters for polymer chain.

Variables	Spring Constant	Number of Beads
Value	500, 5000	20, 50

Variables	L	$\mu L(\frac{\sigma}{\rho\nu})^{0.5}$	Ha Number
Value	25	1	1, 2, 7, 10, 20

Table 3. Setting parameters for magnetic parameter.



**Figure 2.** Comparison of dimensionless velocity profiles of DPD particles (**left**) and dimensionless average velocities (**right**) with analytical results under influence of MHD in simple channel by changing values of *Ha*.

# 3.2. Short Polymer Chain Transfer in MHD Flow

In order to extend the results to the case of polymer translocation in microchannel, the movement of a short no charge polymer chain consisting of 20 beads in a microchannel has been analyzed under influence of MHD flow. Figure 3 illustrates the movement of the polymer chain under different magnetic field strengths (or *Ha*-values) as well as different polymer harmonic bond coefficients

(or spring constants), considering periodic boundary condition at inlet/outlet boundaries. As can be observed, by increasing the *Ha* values from 1 to *Ha* = 20, the relative movement of the short polymer would be more with respect to the hardness coefficient (spring constant) of 500. It has been simulated that conspicuous differences in *x*-direction for the cases of *Ha* = 1 and 20 with the harmonic bond constant of *K* = 500 (red lines with circular symbol and blue lines with diamond symbol) is occurred compared to the cases of *K* = 5000 (green lines with triangle symbols and black lines with gradient symbols). By increasing the harmonic bond constant from 500 to 5000 (10 times), the length of polymers is decreased almost to the half. Results show that choosing the higher *Ha* values and higher harmonic bond constants provides proper polymer chain transfer for low length of polymer cases.



**Figure 3.** Motion of polymer chain with different values for *Ha* parameter and harmonic bond constant (*K*) from number of time steps 1 to 15000 for 20 beads (**left**) and a chain polymer through DPD particles at number of time step 14000 with K = 5000 and Ha = 20 (**right**).

In the following, the effects of magnetic field and hardness of polymers on the properties of polymer chain are investigated. The variation of dimensionless velocity of mass center of the polymer during the time is depicted in the Figure 4 (left). As can be seen, the oscillations decrease over time and, in the case of more severe magnetic field and higher spring coefficient value, the oscillation is greatly reduced. Therefore, in the condition of Ha = 20 and K = 5000 causes the polymer to move with less velocity changes. As is evident from Figure 4 (right), temporal evolutions of the average kinetic temperature for all cases reach to unity and fluid condition approaches the equilibrium. Also, by examining the radius of gyration squared for the polymer chain in Figure 5 (left), it is observed that the amount of distortion and perturbation is greatly reduced around the 80% by increasing the harmonic bond constant from 500 to 5000. Changing the magnetic field has little effect on the polymer chain as shown in Figure 5 (right). Results indicate that in the non-equilibrium situation, the amount of perturbation for a short polymer chain is high for a short period of time, and in the case of higher Ha and K values, low oscillation is resulted for those mentioned parameters. Therefore, again, having a chain with a higher harmonic bond constant has about 80% lower oscillation in this study.



**Figure 4.** Dimensionless velocity of polymer mass center for different *Ha* and *K* values for a polymer chain consisting of 20 beads (**left**) and temporal variation of average kinetic temperature (**right**).



**Figure 5.** Temporal evolution of radius of gyration squared (**left**) and end-end distance (**right**) for different *Ha* and *K* values for a polymer chain consisting of 20 beads.

# 3.3. Long Polymer Chain Transfer in MHD Flow

One of the significant factors in polymer chain transfer is the length of polymer chain. In this study, the effect of MHD is investigated on no charge polymer chain motion and consequently, the length of chain would be influenced from magnetic field. By consideration of previous results, the motion of a polymer chain consisting of 50 beads having different harmonic bond constant values is depicted in Figure 6. As can be expected, higher magnetic field has more effect on the motion in the case of the higher spring constant or K = 5000 compared to K = 500. Also, by increasing the harmonic bond constant, the polymer prefers to collapse and in higher magnetic field, compression is enhanced compared to other conditions. In the maximum circumstance, 40% compression is observed in the case of Ha = 20 and K = 5000. It can be concluded that the proper selection of parameters for transfer of polymer chain are the higher Ha and K values.



**Figure 6.** Motion of polymer chain with different *Ha* parameter and harmonic bond constant (*K*) from time step 1 to time step 15000 for a 50-beads polymer chain (**left**) and a snapshot of polymer chain among DPD particles at time step14000 for K = 5000 and Ha = 50 (**right**).

It can also be concluded from the study of the dimensionless velocity of mass center the rate of velocity variation would greatly decrease as the harmonic bond constant and chain length increase. As Figure 7 indicates, more reduction would be resulted for the magnetic field with Ha = 20 and K = 5000. Similar to the previous results, the average kinetic temperature would converge to unity over the time and fluid would move towards the equilibrium condition. In these cases, for high length of polymer chain, the higher magnetic field and the higher polymer hardness has a proper result.



**Figure 7.** Dimensionless velocity of polymer mass center for different *Ha* and *K* values for a 50-beads polymer chain (**left**) and the temporal evolution of average kinetic temperature (**right**).

By examining the radius of gyration squared and the end-to-end distance, it can be concluded from Figure 8 that a significant decrease of about 75% would occur by increasing the harmonic bond constant from 500 to 5000. It should be noted that higher length of polymer chain delays the equilibrium condition. In this case, higher *Ha* value along with a higher harmonic bond constant present proper polymer chain transfer. In Figure 9, these transfers for both cases of short and long polymer chain with *Ha* = 20 and *K* = 5000 as a high *Ha* and *K* values are shown as a proper polymer chain transfer in this study. For more information from quantity aspect, average properties of radius of gyration squared, dimensionless velocity of polymer mass center, temporal evolution of average kinetic temperature, and the length of polymer chain by consideration of Figure 2 to 8 and different input DPD variable are presented in Table 4. As can be seen again, test case of *Ha* = 20 and *K*=5000 show less perturbation and less strength in polymer chain through transfer in the micro channel.



**Figure 8.** Radius of gyration squared (**left**) and end-end distance (**right**) for different *Ha* and *K* values for a 50-beads polymer chain.



**Figure 9.** Short (N = 20) and long (N = 50) polymer chain transfer in microchannel for Ha = 20 and K = 5000 from number of time steps from 1 to 20000.

Spring Constant	Number of Beads	Ha Number	$\overline{Rg2}$	Vcm	$\overline{T}$	$\overline{N}$
500	20	1	0.54919	0.99985	0.87459	1.5659
5000	20	1	0.11650	1.00033	0.86930	0.7998
500	20	20	0.53191	1.00027	0.86012	1.96924
5000	20	20	0.11838	0.99982	0.87195	0.78627
500	50	1	6.7853	1.00161	0.860313	2.9855
5000	50	1	0.90651	1.00477	0.86932	3.3996
500	50	20	4.3087	0.99984	0.86096	2.7783
5000	50	20	0.85215	0.99985	0.87459	1.8455

**Table 4.** Average values of test cases calculation from number of time steps from 1 to 15000 with different effective input parameters.

#### 4. Conclusions

In this paper, the DPD simulation of a polymer chain through micro channel was investigated by consideration of Magneto Hydro-Dynamics (MHD) body force. The validation of results with analytical solution was presented and accuracy of simulation was in proper range (max. discrepancy was below 10%). Various physical properties of polymer chain in transition were studied, such as radius of gyration squared, velocity of mass center, and average kinetic temperature for short (20 beads) and long polymer chain (50 beads). For all cases, enhancing the *Ha*-value and *K* parameters provide less perturbations for both short and long length of polymer chains, in the case of *Ha* = 20 and *K* = 5000 around the 80% reduction in radius of gyration squared was resulted in this paper.

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