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Simulation of Polymer Chain driven by DPD Solvent Particles in Nanoscale flows

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ABSTRACT

In this study, we simulate the motion and reformation of polymer chain in the nanoscale fluid flow motion of the DPD (Dissipative Particle Dynamics) solvent. The behavior of polymer chain through DPD solvent is studied for 2D and 3D considerations. We implement two body forces of Poiseuille flow and electroosmotic flow to the DPD fluid particles. In case of the electroosmotic flow force, we show that the movement of polymer chain via the electroosmotic phenomenon provides less dispersion than that of the Poiseuille flow for the same polymer chain movement.

1. INTRODUCTION

Dissipative particle dynamics (DPD) is a mesoscopic method that can potentially bridge the gap between atomistic and continuum descriptions in fluids [1, 2]. In biological sciences, there is a growing interest to understand the complex behavior of polymer chain motion in nanochannel. Kong, et al. [3] used the DPD method to simulate polymer beads located in the DPD solvent particles. However, the movement of polymer can be caused in different manners. One of the most important methods, which produces less dispersion, is the electroosmotic flow one. Duong-Hong, et al. [4] used the DPD method to simulate electroosmotic flow in nanochannel for pure DPD particles. They showed that their computational costs are more reasonable comparing with that of the molecular dynamics (MD) method. In this paper, we simulate the motion of polymer chain through Poiseuille flow and electroosmotic flow and show that the electroosmotic flow causes less dispersion for the driven polymer chain.

2. Summary of Electroosmotic Flow (EOF) Theory

The Electroosmotic phenomena can be occurred due to imposing an external electrical field and benefiting from the interaction of ionized solution with the static charges on dielectric surfaces [5]. Consequently, an electric double layer (EDL) is formed close to the solid wall and the interaction of electric field with EDL causes the bulk liquid movement through the microchannels and nanochannels. The EDL influence can be approximately predicted by the Debye length (k^{-1}), which is defined as the distance from the wall. This thickness can be obtained from [6]

$$k^{-1} = (\varepsilon k_B T / 2e^2 z^2 n_\infty)^{1/2} \tag{1}$$

where k_B is the Boltzmann constant, T is the absolute temperature, e is the fundamental charge, z is the valance, n_∞ is the bulk number concentration, h is one-half of the channel height, and ε is the total dielectric constant.

The interaction of the applied electrical field with the positive ions of fluid in the electric double layer generates the electroosmotic flow force. Assuming that the EOF force acts only in the x- direction, we can write

$$F_x = E_0 \rho_e \tag{2}$$

where E_0 is the electrical field and ρ_e is the net charge density in EDL. Using the Poisson equation, the net charge density can be calculated from

$$\varepsilon \frac{d^2\psi}{dy^2} = -\rho_e \tag{3}$$

where Ψ is the electrical potential. Assuming the Boltzmann distribution and considering small zeta-potential magnitudes,

the electrical potential profile can be obtained from the linearized Poisson–Boltzmann equation. It is given by

$$\frac{d^2\psi}{dy^2} = k\psi \tag{4}$$

The distribution of electrical potential can be obtained by implementing the required boundary conditions for the nanochannel case. For the power-law fluid, the viscosity is calculated from

$$\mu = \mu_0 \left(-\frac{dv_x}{dy}\right)^{n-1} \tag{5}$$

where μ_0 is the viscosity of newotonian fluid and n is the flow behavior index. In case of n = 1, the viscous stress becomes a linear function of the rate of strain tensor (newtonian fluid). If n becomes greater than unity, the fluid viscosity increases with the rate of shear stress and if n becomes less than unity (also termed as pseudo plastic), the fluid viscosity decreases as the rate of shear increases.

3. The model

Our model presents the motion of polymer bead through the DPD particles fluid in nanochannel. The DPD particles fluid describes a system of particles having masses of m_i, positions of $\vec{r}_i$, and velocities of $\vec{v}_i$. The resulting interactions are composed of pair wise conservative, dissipative, and random forces exerted on particle i by particle j. These interactions can be summarized into [7]

$$\frac{d\vec{r}_i}{dt} = \vec{v}_i \tag{6a}$$

$$\frac{d\vec{v}_i}{dt} = \sum_{j\neq i} \vec{f}_{ij} + \vec{F}_e \tag{6b}$$

We assume that the mass of particles is normalized to unity. Additionally, $\vec{r}_i$ and $\vec{v}_i$ are the position and velocity vectors. F_e is the external force (electroosmotic force) and $\sum_{j\neq i} \vec{f}_{ij}$ is the internal force to the ith particle by jth particle. The latter force is calculated from

$$\sum_{j\neq i} \vec{f}_{ij} = \sum_{j\neq i} \left[\vec{F}_{ij}^{C} + \vec{F}_{ij}^{D} + \vec{F}_{ij}^{R} \right] \tag{7}$$

where $\vec{F}_{ij}^{C}$ is the conservative force, $\vec{F}_{ij}^{D}$ is the dissipative force, and $\vec{F}_{ij}^{R}$ is the random force. The conservative force is given by

$$\vec{F}_{ij}^{C} = \begin{cases} a_{ij}(1-\mathbf{r}_{ij}/r_c)\vec{r}_{ij} & \mathbf{r}_{ij} < r_c \\ 0 & \mathbf{r}_{ij} \geq r_c \end{cases} \tag{8}$$

where a_{ij} is the maximum repulsion between particles i and j, $\vec{r}_{ij} = (\vec{r}_i - \vec{r}_j)$, $\mathbf{r}_{ij} = \left|\vec{r}_{ij}\right|$, and r_c is a cut-off radius, which is normalized to unity. The dissipating force is given by

$$\vec{F}_{ij}^{d} = -\gamma\omega^D(\mathbf{r}_{ij})(\vec{r}_{ij}\cdot\vec{v}_{ij})(\vec{r}_{ij}) \tag{9}$$

The random force is also given by

$$\vec{F}_{ij}^{R} = \sigma\omega^R(\mathbf{r}_{ij})\theta_{ij}\vec{r}_{ij} \tag{10}$$

where γ, and σ and are the coefficients of the strengths of the dissipative and random forces, respectably. Additionally, ω^R and ω^D are two weight functions and θ_{ij} is a random function having zero mean properties and unit variance. The boundary conditions at the wall consist of two layers of frozen particles and implementing the bounce back condition [8]. The linear polymer chain is described as a chain of M monomers connected by harmonic bonds, whose potential follows the from given by

$$U_{Spring} = \frac{k}{2}\left|\vec{r}_i - \vec{r}_{i-1}\right|^2 \tag{11}$$

If the the spring constant is k = 20. Gyration radius is obtained from [9]

$$\vec{r}_{cm}(t) = \frac{1}{M}\sum_{i=0}^{M} \vec{r}_i(t) \tag{12}$$

$$R_g^2 \equiv \frac{1}{M}\sum_{i=0}^{M} \left\langle \left|\vec{r}_i - \vec{r}_{cm}\right|^2 \right\rangle \tag{13}$$

4. Results and Discussion

In this section, we present the results of our simulation in 2D and 3D**.** We simulate the movement of polymer chain through a pure electroosmotic flow. Table 1 provides the values of constant parameters utilized in the current study. Periodic boundary conditions are applied in the x-direction and z-direction (for 3D) and that an enclose boundary conditions is used in the y-direction [8].

In first step, we verify the DPD solution for Poiseuille flow and newtonian and non-newtonian electroosmotic flows. Figure 1 illustrates the 2D results for the Poiseuille flow case considering constant body force of 0.005. The electroosmotic flow considers a zeta potential of -10 mV, kh=16, and an electrical field of 250 V/m. We consider both newtonian and non-newtonian electroosmotic flow cases with n = 0.8, 1.0, and 1.5. The current numerical velocity profiles are compared with the analytical solution taken from Ref. [6]. To have better comparison with the 2D analytical solutions, we do not introduce any polymer chain into the fluid.

Table 1. The values of constant parameters used in this study

Property	Magnitude	Unit
r_c	1.0	[nm]
a_{ij} (fluid–fluid)	18.75	[N/nm]
a_{wij} (fluid–wall)	5.0	[N/nm]
KbT	1.0	[N/K]
γ	4.5	[N/nm]
z	1.0	[-]
μ_0	9×10^{-3}	[Pa s]
ε	7×10^{-10}	[C/Vm]
n	0.8, 1.5	[-]

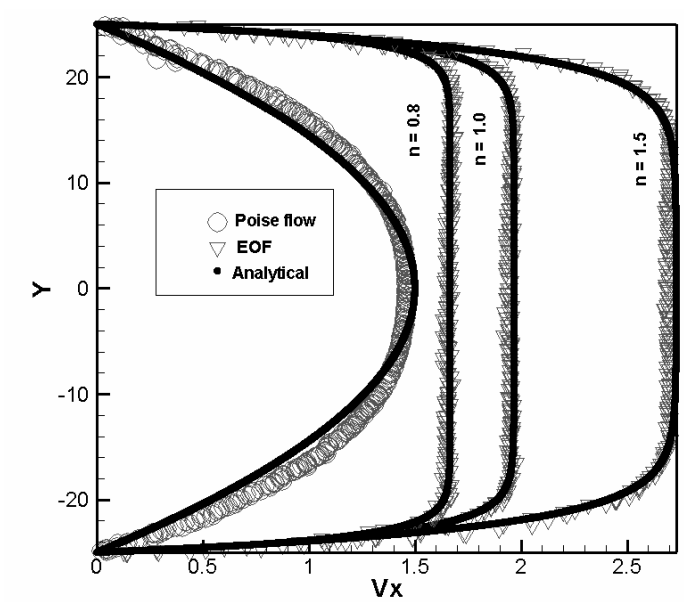
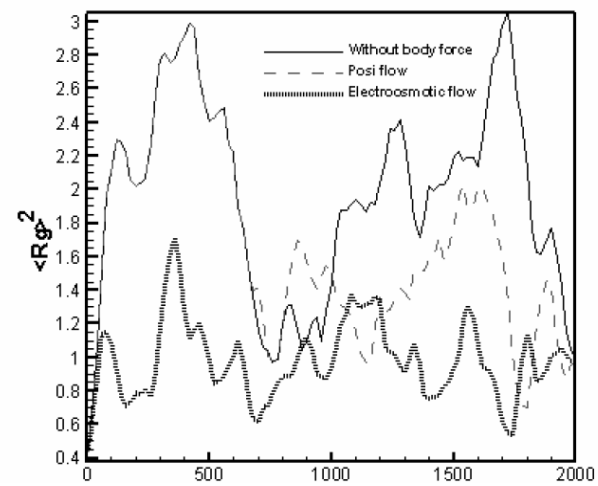
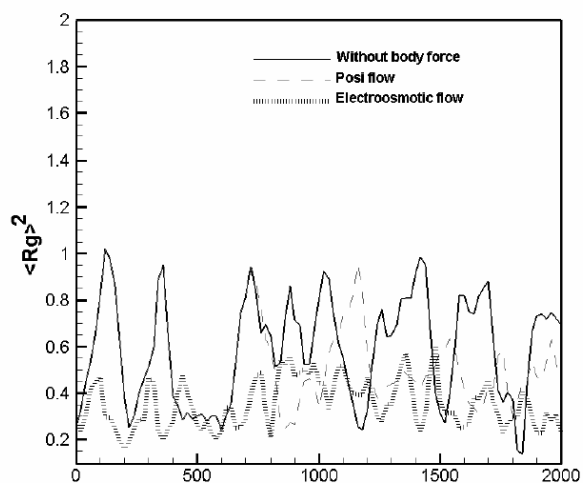


Figure 1. Velocity profiles for 2D EOF and Poiseuille flow and comparing with the theotetical solutions.

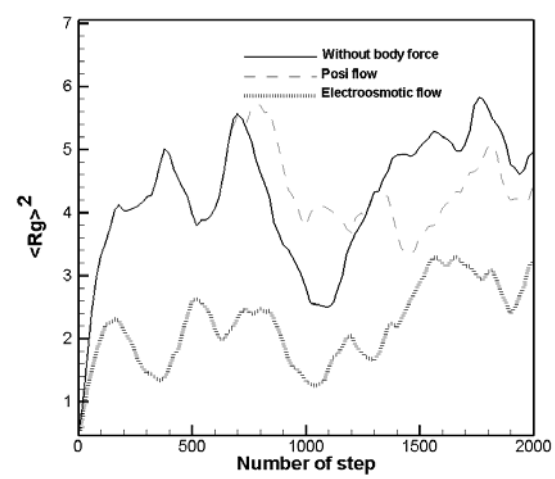
Figure 2 shows the gyration radius variations of polymer chain attending in the fluid without inserting any body forces. The polymer chain is left in Poiseuille flow and also newotonian electroosmotic flow. The study is performed for polymer chain with 5, 10, 20 2D beads. Repulsions between the fluid particles have been chosen 25, between polymer beads and fluid particles is 3 and polymer-polymer beads is 25. As is seen, we have less dispersion polymer chain for the 2D for the case of electroosmotic flow.



a) 5 beads



b) 10 beads



c) 20 beads

Figure 2. Gyration radius variations for 2D polymer chain through time step advancement.

We also simulate the 3D beads in which each chain has more interaction with the fluid particles. Figure 3 shows the gyration radius variations for the polymer chain without enforcing any body force. The polymer movement chain is simulated after inserting in the Poiseuille flow and the newotonian electroosmotic flow. The chain has 20 beads. Again, the results show that the dispersion of polymer chain for the 3D electroosmotic flow is less than that of the Poiseuille flow without inserting any body forces.

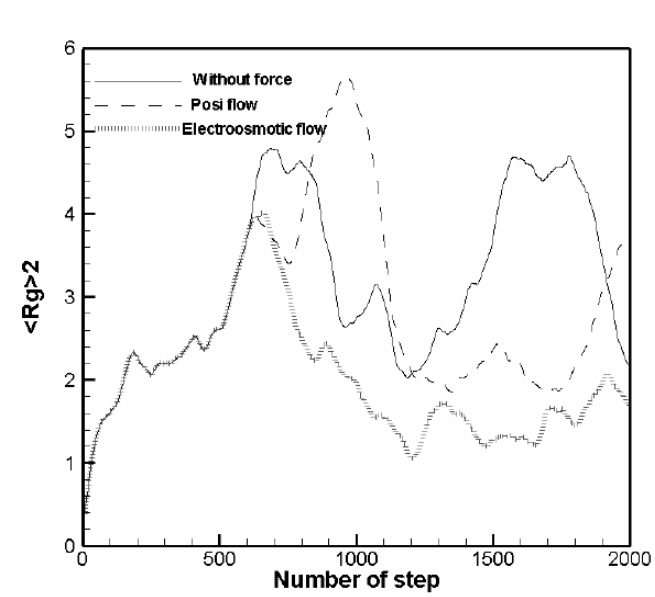


Figure 3. Gyration radius variation for 3D polymer chain through time steps.

Figure 4 shows the changes in 2D of polymer chain shape through nanochannel for a case without inserting body force and during time advancement. It is clear that the polymer chain does not move through the nanochannel because we do not implement any body force.

Figure 5 provides results for the movement of polymer chain through Poiseuille flow in nanochannel. Each bead is affected by the other beads in the polymer chain. The beads are also affected by the DPD particles.

Figure 6 illustrates the result for a polymer chain motion positioned in a newtonian electroosmotic flow. The nanochannel is 2D. Comparing with Figs. 4 and 5, it is clear that the movement of polymer chain through the nanochannel is quite possible. As is seen, we would have less polymer chain dispersion if we use the electroosmotic flow with explained constant parameters.

We also study the chain monometer in 3D cases. Figure 7 provides the results for a case without implementing body force during time advancement. Again, the movement of polymer chain is impossible because there is no body force to drive the polymer beads.

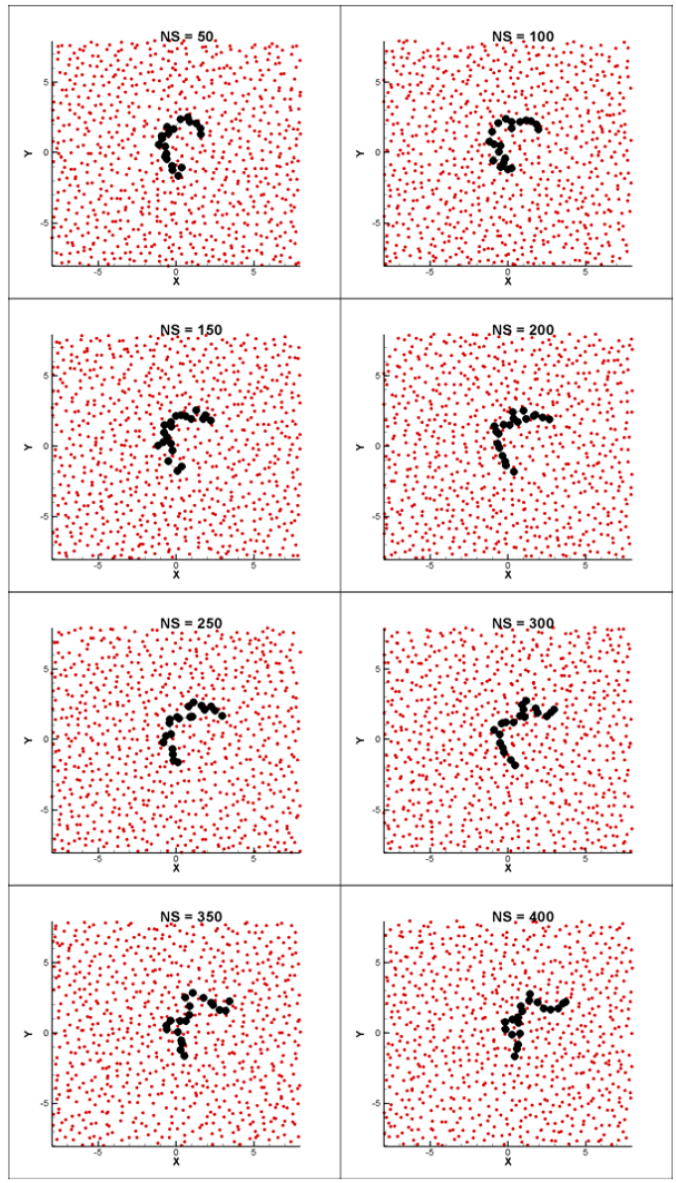


Figure 4. Motion of 2D polymer chain without enforcing any body force and during the time advancement.

Figurer 8 shows the motion of polymer chain by the Poiseuille flow though the nanochannel. Again, the result shows that it is possible the polymer chain inserted in nanochannel with a Poiseuille flow through it.

Figure 9 illustrates the results for the motion of polymer chain inserted in a newtonian electroosmotic flow though a nanochannel considering a 3D simulation. Again, the result shows that it is possible to move the polymer chain through a 3D nanochannel with EOF. Up to here, a comparative study on the results given by Figs. 3, 7, 8, and 9, it is concluded that the electroosmotic phenomenon provides less dispersion for the polymer chain movement.

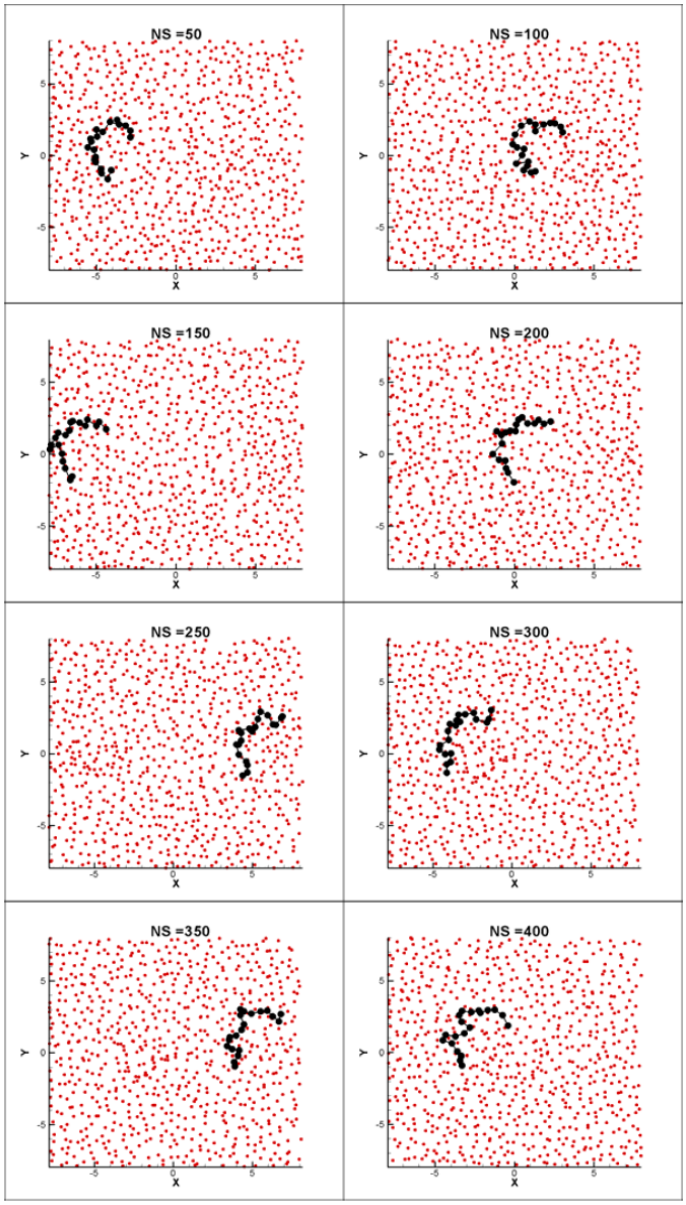


Figure 5. Motion of 2D polymer chain in a Poiseuille flow during the time advancement.

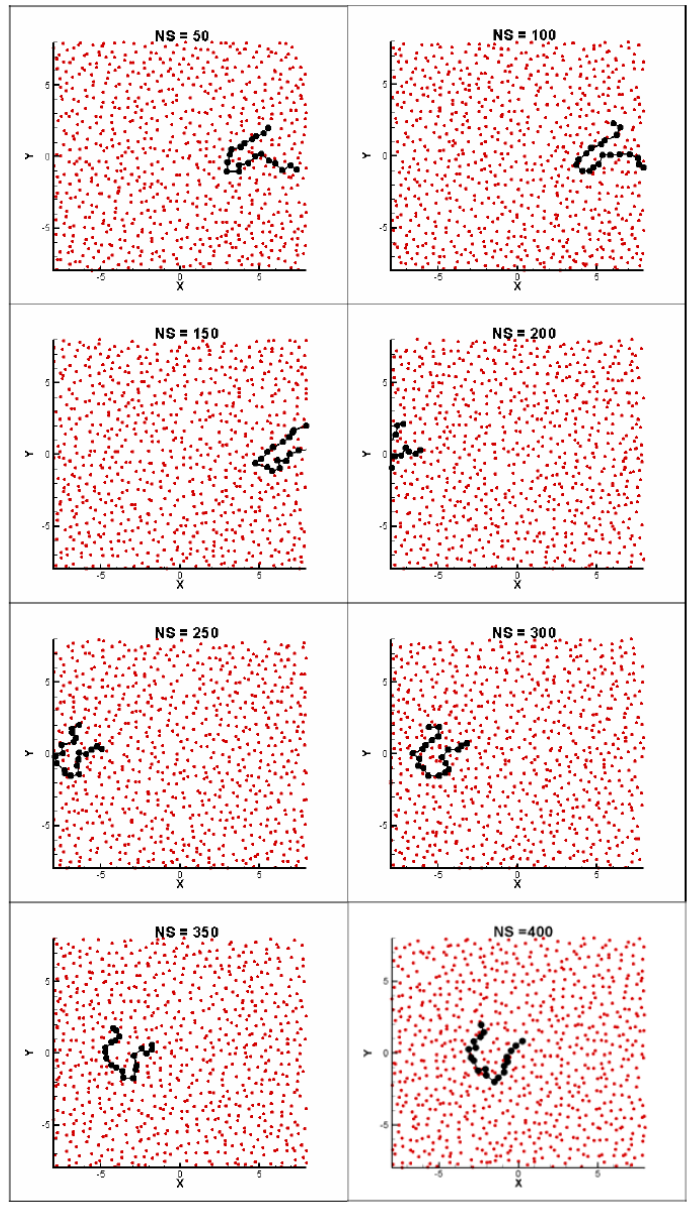


Figure 6. Motion of 2D polymer chain in an EOF during the time advancement.

Ones more, the current results indicate that the prediction of polymer chain movement through the electroosmotic flow, Poiseuille flow and without inserting body force by the DPD method is quite reliable. Additionally, the electroosmotic flow provides less dispersion for a movement of polymer chain in 2D and 3D simulations.

5. Conclusion

We used the DPD method to simulate the motion of polymer chain through Poiseuille flow and newtonian and non newtonian electroosmotic flows. We provided the velocity profiles for the Poiseuille flow and the newtonian and non-newtonian electroosmotic flows without inserting any polymer chain. Our simulations were performed with the motion of polymer chain without any body force and also with body forces in both 2D and 3D cases. Additionally, we simulated the motion of polymer chain by the Poiseuille flow and the

newtonian electroosmotic flow. It was shown that the electroosmotic flow transport the polymer chain with less dispersion than the Poiseuille flow.

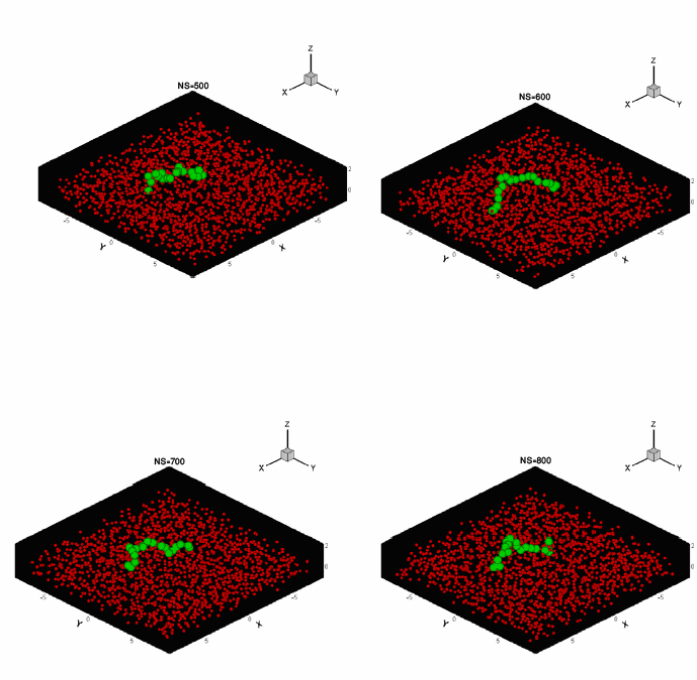


Figure 7. Motion of 3D polymer chain without enforcing any body force during the time advancement.

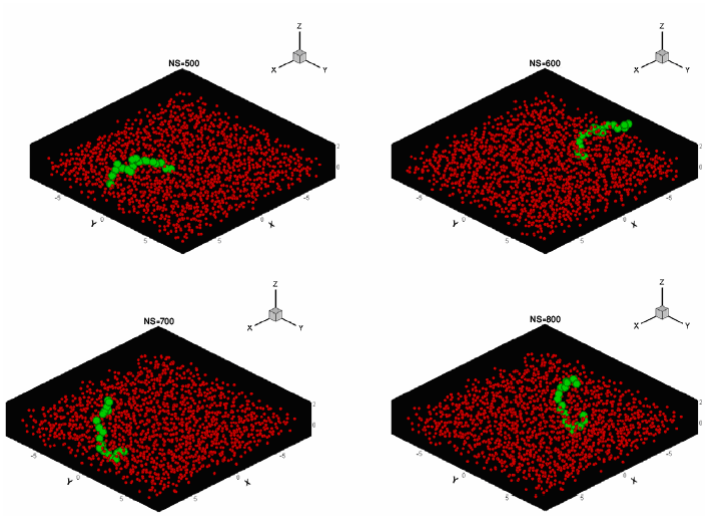


Figure 8. Motion of 3D polymer chain in a Poiseuille flow during the time advancement.

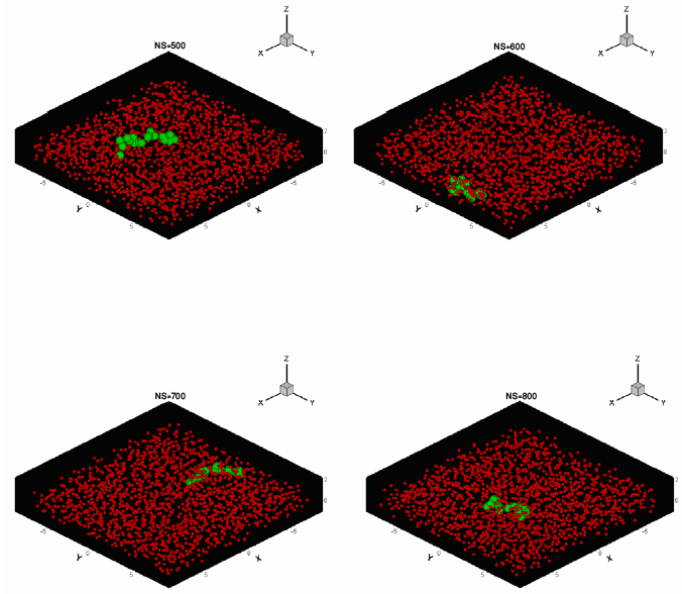


Figure 9. Motion of 3D polymer chain in an EOF during the time advancement.

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