

Brownian Dynamics Simulation of DNA Conformational Trapping in a Micro-Mixing Flow

Abstract

We report that a polymer molecule can be trapped spatially and conformationally using a microflow, which has multiple vortexes. As examples of such a flow, we employed a Taylor vortex flow field, in which the motion of a polymer molecule was simulated using Brownian Dynamics. We find stable conformations of a trapped polymer and determine the conditions for the entrapment and its mechanism.

Introduction

Techniques of single molecule manipulations are becoming essential in the study of biopolymers and in advanced technologies. For example, the trapping and manipulation of DNA molecules using optical traps, micro-pipettes and electric, magnetic, and flow fields are now common. However, all of these trapping methods use some kind of external force.

We report here that a polymer molecule can be trapped both spatially and conformationally using microflows that have at least two stagnation points (or two points with equal velocity) that have a net flow orthogonal to the line connecting them. Such microflows are likely to be common in microdevices in which the velocity gradient varies significantly over the length scale of the polymer. One example considered here is a Taylor vortex velocity field [1] (see Fig. 1). This is an incompressible flow field and can be expressed in terms of a scalar stream function $\phi(x, y)$ as:

$$\phi = \frac{A\alpha^2}{2\pi} \cos(2\pi x / \alpha) \cos(2\pi y / \alpha)$$

$$\begin{cases} V_x = \frac{\partial \phi}{\partial y} = -A\alpha \cos(2\pi x / \alpha) \sin(2\pi y / \alpha) \\ V_y = -\frac{\partial \phi}{\partial x} = A\alpha \sin(2\pi x / \alpha) \cos(2\pi y / \alpha) \end{cases}$$

It is specified by the magnitude of the flow velocity A and the wavelength α .

Method

Using this Taylor vortex velocity field, we compute the three-dimensional motion and deformation of a polymer molecule using the Brownian Dynamics (BD) simulation method. A bead-spring model is employed to represent the polymer molecule, and the following equation of motion is computed for each bead [2]:

$$\mathbf{r}_i(t + \delta t) - \mathbf{r}_i(t) = \mathbf{v}_i(\mathbf{r}_i) \delta t + \frac{\mathbf{f}_i}{\xi} \delta t + \sqrt{\frac{6 \delta t k_B T}{\xi}} \mathbf{n}$$

Here, \mathbf{r}_i and \mathbf{v}_i are the position and velocity vector of bead i (from 0 to $N-1$), respectively, \mathbf{f}_i is the force vector, δt is the time increment of the simulation, ξ is the drag

coefficient of each bead, k_B is the Boltzmann constant, T is the absolute temperature, and \mathbf{n} is a random vector whose components are chosen from the range $[-1, 1]$ in each time step. This is a free-draining BD simulation with hydrodynamic interactions (HIs) between beads ignored.

We also conducted simulations with HI and found that HI hardly changes the results.

The force on each bead is computed by the WLC (worm-like-chain) spring model [3, 4, 5] for the adjacent beads, together with the force from an excluded volume potential between beads. All parameters for the WLC spring model and the excluded volume potential were taken from Ref. [3] to model a λ -DNA molecule.

Results

The simulations show that the molecule can exist in two states, the conformationally trapped and the tumbling state (see Fig. 2). In the tumbling state, the polymer molecule rotates in a vortical region of the flow. In the trapped state, the polymer molecule is held roughly stationary both spatially and conformationally for many polymer relaxation times, even in the presence of Brownian motions.

This phenomenon is analogous to the coexistence of coil-stretch states of a polymer tethered to a plane wall and subjected to a stagnation point flow [6]. In this microflow, the tethered polymer can exist in either a coiled or stretched state, since in the stretched state the free end of the polymer resides in a fast flow that keeps the chain stretched, while in the coiled state, the whole molecule resides near the stagnation point.

A simple local force balance along the molecule between the drag forces from the flow on the beads and the spring forces explains the stability of the trapped state. As shown in Fig. 3, although the drag forces stretch the molecule and tend to pull it upwards, the spring forces acting along the curved contour of the molecule tend to pull the molecule back downwards and limit its stretch. The spring force pulling the molecule toward the center of the curvature is the same force that induces radial migration of a polymer molecule in a curvilinear shearing flow, such as a concentric-cylinder or a cone-and-plate flow [7, 8]. Here, however, the force that connects and stretches the molecule, leading to both conformational and positional trapping, exactly balances this force.

The confinement of a polymer molecule was also found in an electro-osmotic flow field induced in a channel with surfaces with a sinusoidally varying charge (Fig. 4). This effect results from the curved streamline that has a radius of curvature comparable to the polymer molecule size. In micro-/nanochannels that can induce a flow with curved streamlines, such as the micro-well/nanochannel geometry designed by Ohio State University, we may be able to concentrate DNA

molecules utilizing this effect. Future work will be directed towards predicting DNA behavior in these flow fields.

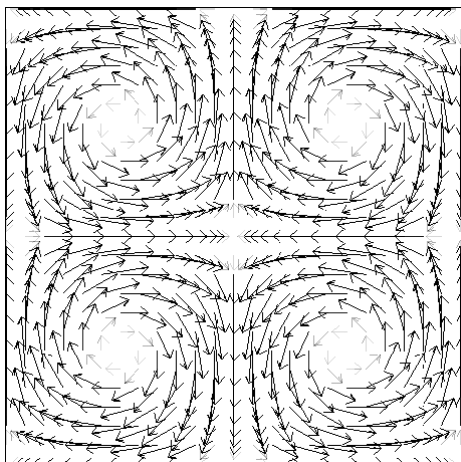


Figure 1. Taylor vortex flow field

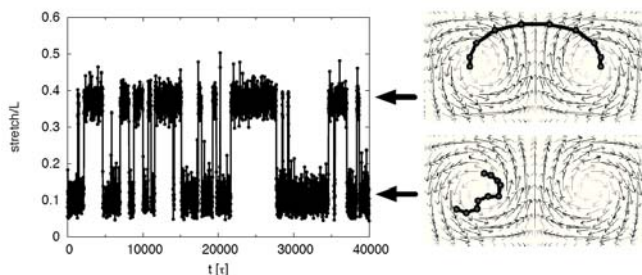


Figure 2. The change of the stretch of a polymer molecule in a Taylor vortex flow of $A\alpha = 2.0[l/\tau]$, $\alpha = 12[l]$ (left). The polymer takes two states: the trapped state (right top) and the tumbling state (right bottom). The polymer molecule has the contour length $21[l]$ (10 beads), and the stretch is defined as the largest distance between beads in a molecule.

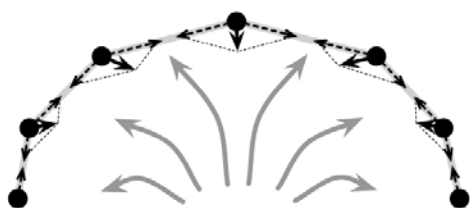


Figure 3. The force balance along curved polymer molecule under fluidic stretching: the spring forces (black arrows) balance the drag forces exerted on beads by a solvent flow (grey arrows)

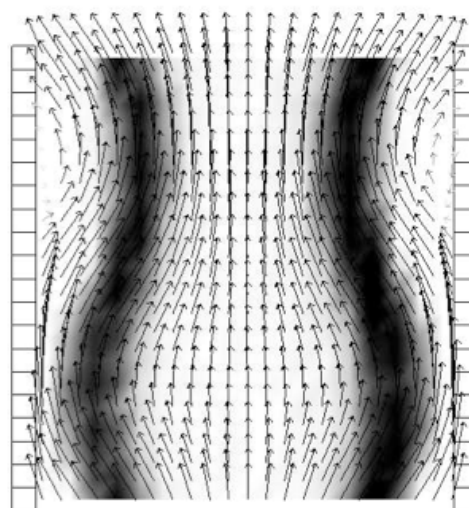


Figure 4. The dark areas represent the distribution of the center-of-mass position of a polymer molecule in an electro-osmotic flow in a channel whose surfaces bear a charge varying sinusoidally plus a net charge: $\sigma(y) = \sigma_0 \cos(qy + \pi/4) + \sigma_{\text{net}}$.

References

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Publications

1. "Fluidic trapping of deformable polymers in microflows" *Nobuhiko Watari, Masao Doi, and Ronald G. Larson* (submitted)