Dynamic Simulation of a Polymer Molecule Using COMSOL Multiphysics: DNA Separation in a Microchannel

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Abstract

In this study, COMSOL Multiphysics was used to simulate DNA separation within a microchannel based on the entropic trapping mechanism. The entropic trapping mechanism involves DNA molecules passing through a series of obstacles in a microchannel and different lengths of DNA exhibiting different elution times from the device based on their entropic tendencies. These lengths of DNA are treated as polymer molecules and can be separated using their elution times. Within COMSOL Multiphysics the Particle Tracing Module was used to perform the Brownian dynamic simulation of a single polymer chain (the DNA chain). The DNA chain was simulated as a bead-chain model where the spring force between each bead was described using the Worm-Like Chain (WLC) model. Bead-bead penetration was prevented by using the Lenard- Jones potential alongside the WLC model. Beads were also considered to be Brownian particles in order to simulate the random motions of the DNA chain as it moves through the solvent within the device. The results from this simulation were then compared with experimental results [e.g. Science (2000) 288, 1026-1029]. Figure 1 shows the simulation of DNA flowing through the microchannel device. This is the first trial, to the best of the authors' knowledge, where COMSOL Multiphysics is used to simulate polymer dynamics. This simulation study will open a new page for the application of COMSOL Multiphysics with polymer dynamics. This in turn will have a positive influence on biomedical applications involving the manipulation of biopolymer molecules.

Figures used in the abstract

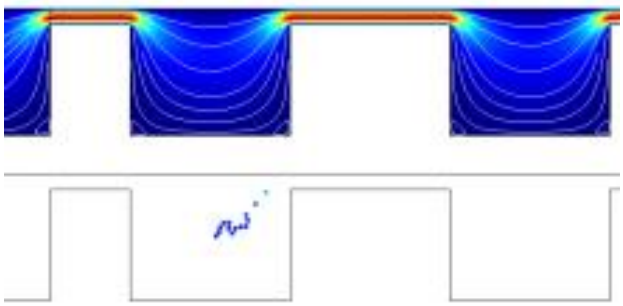

Figure 1: Figure 1. Simulation of DNA flowing through a Microchannel using COMSOL Multiphysics