

The effect of slope in nano-fluidic devices on sieving DNA molecules

*X.Y. Gao¹, J.S. Wang^{2,3}, G.R Liu⁴

1. School of Aeronautics, Northwestern Polytechnical University, Xi'an, P.R. China 710072

2. Singapore-MIT Alliance, E4-04-10, 9 Engineering Drive 1, Singapore 117576

3. Department of Physics, National University of Singapore, 2 Science Drive 3, Singapore 117542

4. School of Aerospace Systems, University of Cincinnati, USA.

*Corresponding author: xygao@nwpu.edu.cn

Nano-fluidic devices are widely employed in the rapidly developing bio-techniques. One of its most interesting applications is sieving particular DNA molecules among others. In a real fabricated nano-fluidic devices, there is usually a minor slope at the ends of each micro-scale pit, this slope do affect the efficiency of DNA sieving. In this paper, with our newly developed dissipative particle dynamics (DPD) simulation algorithm considering both DNA electrophoresis and electroosmotic flows, we numerically investigated the slope effect on DNA sieving in nano-filters. DNA chains are modeled as worm-like chains. The slope is placed at the right side of the nano-filter and the electrical field is applied either forward or backward along the nano-filter. The result shows that DNA chains move in a guided way along the slope. The mobilities of DNA chains increase gradually with the slope angle when DNA chains move up along the slope but decrease with the slope angle when DNA chains move reversely. The later effect is only significant when the slope angle is rather large. The result also shows that there is an optimum angle of the slope for the selected set of DNA chains in simulation where the gradient of mobility vs. DNA length is maximum and thus the sieving effect is the most significant. For short chains, the optimum angle is about 45 degree but for longer chains, the best sieving effect occurs at around 0 degree. It should be noted that, at this circumstance, the mobility might not be desirable. As a result, our simulations suggest that a good nano-filter should be a balance of both effectiveness and efficiency of sieving.

Keywords: Dissipative particle dynamics (DPD) method, DNA electrophoresis, nano-fluidic filter, computer simulation, slope angle, DNA separation.