Macrotransport Model of Bioparticle Separation Using Periodic Micro-Nano Pillar Arrays

*Zirui Li

College of Mechanical and Electrical Engineering, Wenzhou University, China.

*Corresponding author: lizirui@gmail.com

Transport of Brownian bioparticles, such as proteins, DNA and RNA molecules, in porous systems is a fundamental problem in bio-separation processes. Although the so-called free volume model has been a dominant tool for largely qualitative analysis of particle migration since 1970's, it is found that it is accurate only for very small particles (compared with pore sizes) and low electric fields. In more general situations, when the pore size becomes comparable to the particle size, and/or anisotropic particles are involved, the free volume model becomes invalid. Analysis of separation of bioparticles in micro-nano pores has been extremely difficult because of pore randomness and anisotropic particle geometry.

In the past decades, microfabricated devices with periodic regular-shaped nanostructures have been successfully used for biomolecular separation[1]. Apart from their significant success in engineering aspects, such devices also provide a superior platform for theoretical investigation of the fundamental mechanism because of accurate control over the device geometry.

In this abstract, we report a theoretical modeling of electrophoretic migration of biomolecules in periodic nano-pillar arrays as shown in Fig. 1. The key separation mechanism in such devices derives from steric constraints on the molecules' configurational freedom(an entropy barrier). Molecular separation occurs because of different barrier heights for different molecules, which produce different effective migration speeds. Simpler systems have been studied theoretically using various approaches, including empirical formulation, stochastic particle simulation methods (such as Brownian dynamics and dissipative particle dynamics), and continuum modeling[2,3], etc. However, molecular migration in the periodically arranged micro-nano arrays is too difficult for these simulation techniques due to extremely heavy computational requirement. Here, we use macrotransport theory to calculate accurate phenomenological molecular mobility and diffusivity, without expensive stochastic simulation or modeling of large, repeated structures. Actually, steady state solution of probability distribution over one single unit of micro-nano array is required instead of transient analysis of molecular migration over a huge number of repeats of micro-nano units.

Keywords: Biomolecular separation; Macrotransport model; Electrophoresis



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