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RESEARCH PAPER

Simulation of mixed electroosmotic/pressure-driven flows by utilizing dissipative particle dynamics

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Abstract In this paper, we present an extension of dissipative particle dynamics method in order to study the mixed electroosmotic/pressure-driven micro- or nano-flows. This method is based on the Poisson–Boltzmann equation and has a great potential to resolve the electric double layer (EDL). Hence, apart from studying the bulk flow, it also provides a strong capability in order to resolve the complex phenomena occur inside the EDL. We utilize the proposed method to study the pure electroosmotic and also the mixed electroosmotic/pressure-driven flow through the straight micro-/nano-channels. The obtained results are in good agreement with the available analytical solutions. Furthermore, we study the electroosmotic flow and motion of DNA molecules through a T-shaped micro-channel. We show that neglecting the EDL and utilizing the slip wall boundary condition model can result in crucially misleading hydrodynamic characteristics if the EDL is comparable to the width of the channel. Finally, we utilize the presented method in order to study the complex flow patterns, which are created due to the heterogeneous distribution of the electric potential of the walls. These complex flow patterns usually are utilized in order to enhance the efficiency of mixing process in micro-/nano-length scales. In addition, we show that they can also be utilized effectively in order to separate the different macromolecules such as polymers, DNA molecules and so on, according to their length of chain.

Keywords Mixed electroosmotic/pressure-driven flow · Electric double layer · Dissipative particle dynamics · MEMS · NEMS · DNA molecular sieving

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1 Introduction

Micro- and nano-fluidic flows have attracted a great amount of interests in the last decades thanks to the technology advances, which have enabled the researchers to fabricate the miniaturized devices in order to achieve a wide variety of different goals in bio-analysis, cell biology, chemical synthesis, pumping, separation, mixing and so on (Mishchuk et al. 2011; Zhu et al. 2011; Liu et al. 2004; Viovy 2000). Since the surface-to-volume ratio increases dramatically in the micro- and nano-devices, the transportation phenomena can take place more efficiently. Considering this fact enables us to achieve the high-performance devices such as pumps, mixers, separators and so on.

It is by no means possible to say which of the electroosmotic flow (EOF) or the pressure-driven flow (PDF) mechanisms is more efficient. Each of them has its own advantages and disadvantages, and consequently its own applications. The very small width of the micro- or nano-channels results in large pressure differences to be required for making the fluid flow. Hence, fabrication of the corresponding systems, especially those with moving components, has significant difficulties. In addition, the high-pressure values that are sometimes required in pressure-driven devices can damage the chip itself, if the PDF is utilized for a lab-on-a-chip (LOC) (McMahon 2007). Furthermore, one of the most important disadvantages of PDF

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