COMMUNICATIONS IN COMPUTATIONAL PHYSICS
Vol. **2**, No. 6, pp. 1055-1070

Commun. Comput. Phys.
December 2007

Lattice Poisson-Boltzmann Simulations of Electroosmotic Flows in Charged Anisotropic Porous Media

Moran Wang[1,2,*], Ning Pan[1], Jinku Wang[3] and Shiyi Chen[2,4]

[1] *Department of Biological & Agricultural Engineering, University of California, Davis, CA 95616, USA.*
[2] *Department of Mechanical Engineering, Johns Hopkins University, Baltimore, MD 21218, USA.*
[3] *School of Aerospace, Tsinghua University, Beijing, China.*
[4] *College of Engineering, Peking University, Beijing, China.*

Received 7 November 2006; Accepted (in revised version) 7 March 2007

Available online 15 June 2007

Abstract. This paper presents numerical analysis of electroosmotic flows (EOF) in charged anisotropic porous media using the lattice Poisson-Boltzmann method (LPBM), which combines two sets of lattice evolution methods solving the nonlinear Poisson equation for electric potential distribution and the Navier-Stokes equations for fluid flow respectively. Consistent boundary condition implementations are proposed for solving both the electrodynamics and the hydrodynamics on a same grid set. The anisotropic structure effects on EOF characteristics are therefore studied by modeling the electrically driven flows through ellipse arrays packed in a microchannel whose shape and orientation angle are used to control the anisotropy of porous media. The results show that flow rates increase with the axis length along the external electric field direction for a certain porosity and decrease with the angle between the semimajor axis and the bulk flow direction when the orientation angle is smaller than $\pi/2$. After introducing random factors into the microstructures of porous media, the statistical results of flow rate show that the anisotropy of microstructure decreases the permeability of EOFs in porous media.

PACS (2006): 47.56.+r; 47.57.jd

Key words: Electroosmotic flow, anisotropic porous media, lattice Poisson-Boltzmann method.

1 Introduction

Electroosmotic flows (EOF) in porous media have been studied for nearly two hundred years due to their important applications in soil, petroleum and chemical engineering

*Corresponding author. *Email addresses:* `mmwang@ucdavis.edu` (M. R. Wang), `npan@ucdavis.edu` (N. Pan), `wjk01@mails.tsinghua.edu.cn` (J. K. Wang), `syc@jhu.edu` (S. Y. Chen)

since the electrokinetic effects were first observed by Reuss in 1809 in an experimental investigation on porous clay [1-3]. In the past few decades, there are considerable and reawakening interests in the EOF in porous media because of the conspicuous applications in biological-chemical-medical analysis [4-6] and new techniques in energy and geophysical engineering [7,8], especially in micro- and nanoscales. Recently, charged porous structures have been employed in some devices to control and improve the fluid behavior as expected. Microparticles which are packed in microchannels have been used to improve the performances of electroosmotic micropumps with a lower flow rate and a higher pumping pressure [9-11]. Owing to the polarization effect of porous electrodes, the structured electrode arrays have been designed as a concentration demixer of electrolytes [12].

The EOF dynamics in porous media has been studied much both theoretically [13-20] and numerically [20-29]. By improving the simple capillary tube model [13], Mehta and Morse [14] schematized a micro porous membrane by an array of charged uniform spheres. Jin and Sharma [16] extended the capillary model to two-dimensional square lattice network model, which is more appropriate in simulating inhomogeneous porous media. Grimes et al. [18] developed the cubic lattice network of interconnected cylindrical pores model and simulated the intraparticle electroosmotic volumetric flow rate and velocity in the three-dimensional pore network of interconnected cylindrical pores. Generally, the theoretical models can give an overall prediction of the EOF characteristics, but few can present flow structure details. Besides the various theoretical models, pure numerical methods have been developed in the past decade for predicting details of EOF in porous media owing to the rapid developments of computer and computational techniques [20-28]. The premier efforts of the numerical predictions for the EOF in porous media focused on the linearized model of nonlinear governing equation for electric potential distribution due to the numerical instability and time-consuming characteristic of solving the original nonlinear Poisson-Boltzmann equation [20-25]. However, both experimental data and the first principle analysis have indicated that when the zeta potential is greater than 30 mV the linear assumption of the Poisson-Boltzmann equation will break down [29,30].

Hlushkou et al. [26] proposed a numerical scheme for modeling the EOF in porous media, which involves a traditional finite-difference method (FDM) for solving the nonlinear Poisson-Nernst-Planck equations for electrodynamics and a lattice Boltzmann method (LBM) for Navier-Stokes equations for hydrodynamics. The coupled methods have been used to investigate the flow fields between random arrays of spheres [27] and in colloids systems [28]. Almost at the same time, Wang et al. [31,32] presented a lattice Poisson-Boltzmann method (LPBM) for predicting the EOF in microchannels, which combines a lattice Poisson method (LPM) for solving the nonlinear Poisson equation for electric potential distribution with a lattice Boltzmann method (LBM) for solving the Boltzmann-BGK equations for fluid flow. The LPBM has been employed to analyze the mixing enhancement by EOF in microchannels [33] and the improved pumping performances by the changed isotropic porous media additives in micropumps [34]. To our