마이크로체널에서의 EOF에 대한 Nernst-Planck 모델과 Poisson-Boltzmann 모델의 비교

김태원, 이원민, 최영진, 박흥목*
서강대학교 화공생명공학과
(hmpark@sogang.ac.kr*)

Comparison of the Nernst-Planck model and the Poisson-Boltzmann model for the electroosmotic flows in microchannels

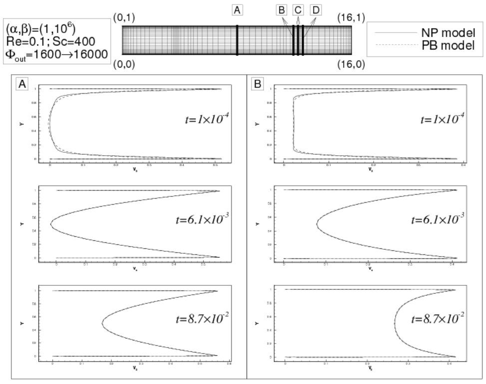
T.W. Kim, W. M. Lee, Y. J. Choi, H. M. Park*
Department of Chemical and Biomolecular Engineering, Sogang University
(hmpark@sogang.ac.kr*)

1. Introduction

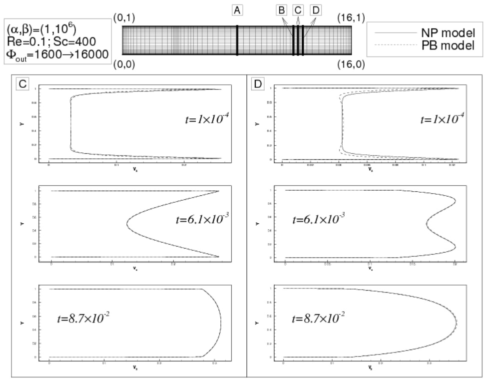
In the most analysis of electroosmotic flows, the ionic distribution in the electric double layer is assumed to follow the equilibrium Boltzmann distribution, resulting in the Poisson-Boltzmann equation for the electric potential induced by theses ions. However, the convective transport of these ions may have significant effects in certain technologically important cases. We may mention the electroosmotic flows through a sudden expansion or a sudden contraction, where the streamlines deviates from the rectilinear ones. Other important cases are flows through a microchannel with inhomogeneous distribution of zeta potential which may induce local vortex ow, or electroosmotic flow through a narrow microchannel where the electric double layer overlaps around the center of the channel. In these cases, the Boltzmann equation is not valid for the ionic distribution and the Nernst-Planck equation has to be employed to find a more exact distribution of ions in the electric double layer. In the present investigation, we shall compare the velocity profiles obtained from the Nernst-Planck equation with those from the Poisson-Boltzmann equation for these cases and examine how the difference in the predicted velocity fields from these two equations affects the predicted solute transport and residence time in the microchannels.

2. Results

Figs.1a,b show the comparison of axial velocity v_x obtained from the PB model with that from the NP model for $(\alpha, \beta) = (1, 10^6)$ at the axial locations A, B, C and D indicated in the same figure at various instants when out changes from 1600 to 16000 at t = 0. The dimensionless zeta potential is 1.0 until the location B and decreases to zero at the location D linearly. Thus is 0.5 at the location C. It is expected that the effect of inhomogeneous zeta potential may occur near the locations B, C and D, while the velocity prole around the location A is affected by the homogeneous zeta potential. It is shown that at all locations the predictions from the PB model are almost the same as those from the NP model. In this case, the electric double layer is so thin that the ions follows the Boltzmann distribution closely.

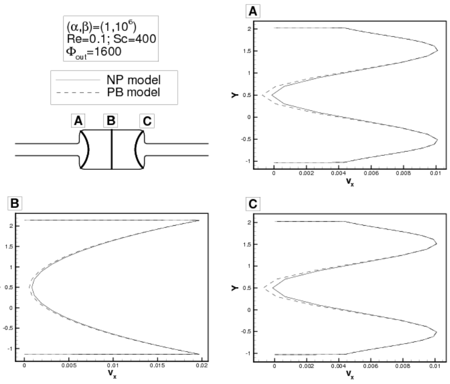


<Fig1a>

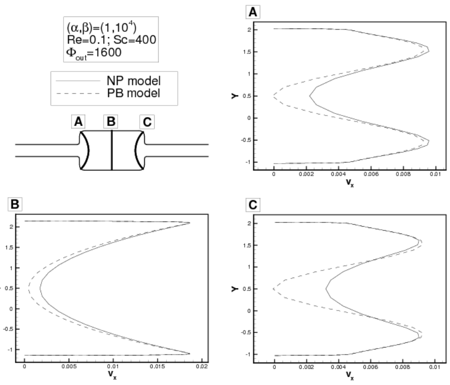


<Fig1b>

Next consideration is the electroosmotic flow through an irregular shaped channel where the contribution of convective transport of ions, i.e., $\mathbf{v} \cdot \nabla n^{\pm}$ in equations (1)-(2), may be significant. Figs.2a,b show the comparison of the steady state axial velocity from the PB model and that from the NP model at the three locations, A, B and C, indicated in the same figure when $\phi_{out} = 1600$ for the two cases of $(\alpha, \beta) = (1, 10^6)$ and $(\alpha, \beta) = (1, 10^4)$. It is shown that there is a significant discrepancy between the velocity from the PB model and that from NP model when the electric double layer is thick, i.e., $(\alpha, \beta) = (1, 10^4)$ although the two models predict similar velocity fields for $(\alpha, \beta) = (1, 10^6)$ where the electric double layer is very thin. For example, the PB model predicts that a recirculating ow starts to appear near the center of the chamber, i.e., $v_x \leq 0$, for the case of $(\alpha, \beta) = (1, 10^6)$, whereas the NP model does not predict any recirculating ow at the same region.

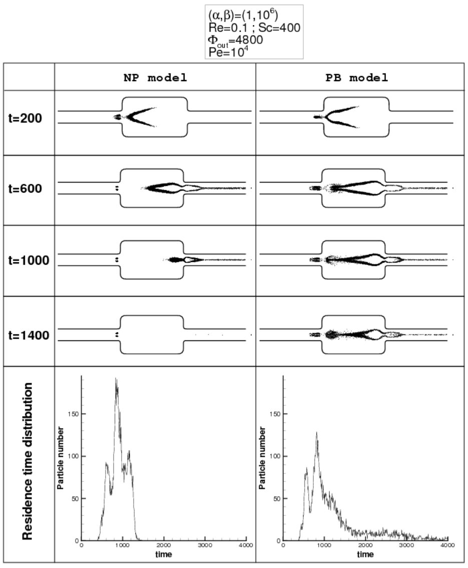


<Fig2a>



<Fig2b>

Finally we investigate how the difference in the velocity fields from these two models affects the predicted solute transport through the irregular microchannel.



<Fig3>

3. References

[1] D. J. Harrison, Z. A. Man, Z. Fan and H. M. Widmer 1992 Capillary electophoresis and sample injection systems integrated on a planar glass chip. Anal. Chem. 64, 1926-32.

[2] A. Moldavan 1934 Science 80, 188.

[3] C. S. Eerhauser, A. Paulus, Z. A. Man and H. M. Widmer 1994 High-speed separation of antisence oligonucleotides on a micromachined capillary electophoresis device. Anal. Chem. 66, 2943-53.

[4] V. Srinirasan, V. K. Pamula and R. B. Fair 2004 An integrated digital microfluidic lab-on-a-chip for clinical diagnostics on human physiological fluids. Lab. Chip 4, 310-5.

[5] C-Y Lee, G-B Lee, J-L Lin, F-C Huang and C-S Liao 2005 Integrated microfluidic systems for cell lysis, mixing/pumping and DNA amplification. J. Micromech. Microeng. 15, 1215-23.

[6] M. J. Pugia, G. Blankenstein, R-P Peters, J. A. Prott, K. Kadel, T. Willuis, R. Sommer, H. H. Kuo and L. S. Schulman 2005 Microfluidic tool box as technology platform for hand-held diagnosis. Clin. Chem. 51, 1923-32.

[7] E. T. Lagally, I. Medintz and R. A Mathies 2001 Single-molecule DNA amplification and analysis in an integrated microfluidic device. Anal. Chem. 73, 565-70.

[8] R. F. Probstein, Physicochemical Hydrodynamics. Wiley, NewYork, 1994.

[9] R. J. Yang, L. M. Fu and Y. C. Lin 2001 Electroosmotic flow in microchannels. J. Colloid Interface Sci. 239, 98-105.

[10] R. J. Yang, L. M. Fu and C. C. Hwang 2001 Electroosmotic entry flow in a microchannel. J. Colloid Interface Sci. 244, 173-79.

[11] H. Keh and Y. C. Lin 1995 Electrokinetic ow in a circular capillary with a surface charge layer. J. Colloid Interface Sci. 172, 222-229.

[12] L-M Fu, J-Y Lin and R-J Yang 2003 Analysis of electroosmotic flow with step change in zeta potential. J. Colloid Interface Sci. 258, 266-275.

[13] H. Keh and H. C. Tseug 2001 Transient electrokinetic flow in fine capil laries. J. Colloid Interface Sci. 242, 450-459.

[14] T. J. Johnson, D. Ross, M. Gatan and L. E. Locascio 2001 Laser modification of preformed polymer microchannels: application to reduce band broadening around turns subject to electrokinetic ow. Anal. Chem. 73, 3656-3661.

[15] M. M. Rahman and T. Siikonen 2000 An improved simple method on a collocated grid. Numer. Heat Transfer Part B: Fundamentals 38, 177-201.