전기삼투흐름에서 비균일 제타 포텐셜의 측정

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Estimation of inhomogeneous zeta potential using velocity measurements in the electroosmotic flow

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1. Formulation of problem

We consider a simple electrolyte that dissociates into two equally charged ions of valence z and -z. The electric potential in the electric double layer, induced by these ions, is governed by the following Poisson-Boltzmann equation [1].

$$\nabla^2 \psi = -\frac{4\pi \rho_e}{\varepsilon_0 \varepsilon}$$

Hence, ψ is the electric potential, ρ_e is the net charge density, ϵ_0 is the permittivity of vacuum and ϵ is the dielectric constant. The net charge density ρ_e is given by

$$\rho_e = -2zen_0 \sinh\left(\frac{ze\psi}{k_BT}\right)$$

where n_0 is the bulk ionic concentration, k_B is the Boltzmann constant, and T is the absolute temperature. The electroosmotic flow is created by applying an external electric field $-\nabla \phi$ in the streamwise direction. Then the total electric field, $-\nabla \psi - \nabla \phi$, interacts with the ions in the electric double layer and creates an electrokinetic body force. The corresponding Navier-Stokes equation with the electrokinetic body force is as follows.

$$\rho_f \left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right) = -\nabla P + \mu \nabla^2 \mathbf{v} + 2zen_0 \sinh\left(\frac{ze\psi}{k_B T}\right) (\nabla \psi + \nabla \phi)$$

$$\nabla \cdot \mathbf{v} = 0$$

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2. Result

The conjugate gradient iteration is terminated as soon as the value of the performance function J becomes less than ϵ^2_{er} . Fig.1-a and Fig.1-b show the estimated profiles with the corresponding estimation error and iteration numbers for the case of 5% measurement error and 10% measurement error, respectively, while the other conditions are the same as those in Fig.2. Although the estimation error increases with the measurement error, it is shown that the present method estimates the zeta potential reasonably even with the noisy measurements. It is expected that we may estimate more complicated ζ profiles with the increased number of measurement locations. Fig.3 shows the estimation of somewhat complicated profile with ten measurements locations. On the other hand, the simultaneous estimation of the zeta potential at the upper and near the lower wall.

3. Conclusion

The accurate measurement of zeta potential is one of the most important prerequisites in the design and operation of microfluidic systems. In the present work we have devised a method of estimating the zeta potential using simulated velocity measurements in microchannels. Employing a conjugate gradient method, which alleviates the difficulties associated with the ill-posedness, it is demonstrated that we can determine the zeta potential accurately even with noisy velocity measurements. The heterogeneous potential occurs due to the adhesion of protein to the channel walls unintentionally. Sometimes it is introduced intentionally by chemical surface modification to induce secondary flow or to diminish the turn-induced band broadening. In these cases, the zeta potential distribution can be determined efficiently using the present technique.

4. Reference

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Figure 1. Effect of measurement error. (a) 5% error, (b) 10% error.



Figure 2. Estimation of ζ at the upper wall of the 2–D straight channel.

 $(\alpha = 4.0, \beta = 10^6, Re = 0.1).$

- (a) Five measurement locations.
- (b) Performance function with respect to the iteration number.
- (c) Estimated $\,\zeta\,$ profile at certain iteration number.
- (d) Comparison of the exact (correct) ζ and the converged estimation.

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Figure 3. Estimation of a complicated ζ profile with ten measurement locations.