電解質溶液在表面覆蓋離子可穿透薄膜之微管中的流動

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一、中文摘要
本研究中考慮電解質溶液在表面覆蓋離子可穿透薄膜之橢圓微管中流動現象。文中探討系統之體積流率、總電流、電黏度效應與流場電位。結果顯示當中離子強度時，這些量為幾何形狀比之函數，且有一極大或極小值。此現象在一表面無覆蓋離子可穿透薄膜之橢圓微管中並無出現。

關鍵詞: 微流管, 電動力現象, 電黏滯效應, 幾何形狀比

Abstract
The electrokinetic flow of an electrolyte solution in an elliptical microchannel covered by an ion-penetrable charged membrane layer is examined theoretically. The present analysis extends previous results in that a two-dimensional problem is considered. The system under consideration simulates the flow of a fluid, for example, in vein. The electroosmotic volumetric flow rate, the total electric current, the streaming potential, and the electroviscous effect of the system under consideration are evaluated. We show that, for a constant hydraulic diameter, the variations of these quantities as a function of the aspect ratio of the microchannel may have a local minimum or a local maximum at a medium level of ionic strength, which depends on the thickness of the membrane layer. For a constant cross-sectional area, the electroosmotic volumetric flow rate, the total electric current, and the streaming potential increase monotonically with an increase in the aspect ratio. The electroviscous effect decreases monotonically with an increase in the aspect ratio.

Keywords: microchannel, electrokinetic phenomenon, electroviscous effect, aspect ratio

二、緣起與目的
Due to its versatile applications in practice, the electrokinetic phenomenon in a microchannel has drawn the attention of many researches recently. In contrast to that in the case of a macrochannel, the flow of fluid in a microchannel is influenced significantly by the charged conditions on channel wall, an the corresponding governing equations need to be modified accordingly. Burgreen and Nakache1 examined the electrokinetic phenomenon in an ultrafine rectangle microchannal under the conditions of large electrokinetic radius or low surface potential. Assuming Debye-Huckel condition, Rice and Whitehead2 discussed the influence of the electrokinetic radius on the electrokinetic flow in a narrow cylindrical channel. Sørensen and Koefoed3 analyzed the electrokinetic flow in a rigid cylindrical channel for the case of fixed surface charge density under Debye-Huckel condition. Their analysis was extended by Keh and Liu4 to the case the channel wall is covered by an ion-penetrable layer containing fixed charge. Recent observations reveal that assuming a rigid wall is unrealistic to some microchannel. Ohshima and Ohki6 proposed using a model in which a rigid surface is covered by an ion-penetrable membrane layer. The latter contains a uniformly distributed fixed charge. It was concluded that the ion-penetrable membrane layer plays a significant role in determining the behavior of the whole system. Donath and Voigt7 examined the electrokinetic flow in a planar slit, the surface of which is covered by an...
ion-penetrable layer. Under specified fixed charge distribution, they were able to derive an analytic solution for the governing nonlinear Poisson-Boltzmann equation, and numerical solutions were presented for a general fixed charge distribution. The applicability of the results obtained were justified by experimental observations. Ohshima and Kondo\(^8\) considered the electrokinetic flow in a planar slit covered by an ion-penetrable membrane layer. Under the conditions of uniform fixed charge distribution and large separation distance between two plane, they were able to derive analytical expressions for the electroosmotic velocity, volumetric flow rate, and total current. Their analysis was extended by Tseng et al.\(^9\) to a more general condition. Hsu and Kao\(^10\) investigated the electroosmosis in a rectangle microchannel covered by an ion-penetrable membrane layer. It was found that the electrokinetic behavior of the geometry considered is influenced significantly by the aspect ratio of the microchannel. In particular, at a medium ionic strength, a local maximum or a local minimum may present as the thickness of the ion-penetrable membrane layer varies. Yang et al.\(^11\) analyzed the electroosmosis in a planar slit with a 90° elbow. They found that if Reynolds number is large, separation bubble can be detected near the 90° elbow. Hsu and Kao\(^12\) studied the electrokinetic flow in a rigid spheroidal tube. Yang and Kwok\(^13\) studied the flow in a cylindrical microchannel. The influence of electrokinetic force and Navier’s slip condition were considered, and an analytical solution for the oscillating flow was obtained.

In this study the flow of an electrolyte solution in a spheroidal microchannel covered by an ion-penetrable membrane is investigated. We extend previous analyses in that a microchannel with a non-rigid surface and a spheroidal cross sections is considered. The influences of the key parameters on the electrokinetic flow under consideration are discussed through numerical simulation. These include the ionic strength, the thickness of membrane layer, and the geometry of a channel.

三、理論

We consider a steady flow of an \(a:b\) electrolyte solution, \(a\) and \(b\) being respectively the valences of cations and anions, in an elliptic microchannel of length \(L\), major axis \(2W\), and minor axis \(2H\). The surface of the microchannel is covered by an ion-penetrable membrane layer of thickness \(d\), which carries fixed charge. Suppose that \(L\) is sufficiently long so that the end effects can be neglected. The Cartesian coordinates \((x,y,z)\) are adopted with its origin located at the center of the microchannel. Because the flow of liquid is in the \(z\)-direction, only the \(z\)-component of fluid velocity \(V\), \(u(x,y)\), needs to be considered. An electric field \(E_z\) with magnitude \(E_z = -\frac{\partial \psi}{\partial z}\) in the \(z\)-direction is applied, and a pressure gradient \(P\) with magnitude \(P = -\frac{\partial \psi}{\partial z}\) in the same direction, where \(\psi\) and \(p\) are respectively the electrical potential and the pressure. The liquid phase, which contains an \(a:b\) electrolyte, has constant dielectric constant \(\varepsilon\) and viscosity \(\eta\). As illustrated in Figure 1(b), the symmetric nature of the present problem suggests that only the quarter of the cross section of the microchannel,

\[
\Omega = \{ x^2/W^2 + y^2/H^2 \leq 1 \middle| \ x \geq 0 \ \ y \geq 0 \} ,
\]

needs to be considered. In Figure 1(b), \(\Omega_1\), \(\Omega_2\), and \(\Omega_3\) are the boundaries of \(\Omega\), and \(\Omega_4\) represent the membrane-liquid phase interface.

The electric potential \(\psi(x,y,z)\) comprises that arising from the applied electric field \(-E_z z\) and that arising from the charged membrane \(\phi(x,y)\). We have

\[
\psi(x,y,z) = \phi(x,y) - E_z z
\]

\(\phi(x,y)\) can be described by

\[
\text{(1)}
\]
where $C_0$ is density of fixed charge in the membrane layer and $w$ is its valence, $\rho_{el}$ is the space charge density of mobile ions, and $j$ is a region index ($j=0$ for liquid phase, $j=1$ for membrane layer). We assume that both $C_a$ and $C_b$ follow a Boltzmann distribution, that is,

$$\begin{align*}
C_a &= C^0_a \exp(-aF\phi/RT) \\
C_b &= C^0_b \exp(bF\phi/RT)
\end{align*}$$

where $C^0_a$ and $C^0_b$ are respectively the bulk concentrations of cations and anions, $F$ and $R$ are respectively the Faraday constant and the gas constant, and $T$ is the absolute temperature. Applying the electroneutrality condition $aC^0_a = bC^0_b$, the space charge density for mobile ions $\rho_{el}$ can be expressed as

$$\rho_{el} = -aC^0_a F[\exp(bF\phi/RT) - \exp(-aF\phi/RT)]$$

Therefore eq (2) becomes

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = -\left(p_{el} + jwFC\right) \frac{1}{\varepsilon} \quad \Omega \in \mathbb{Y}, \mathbb{X} \quad \Omega_4^+ = \phi \Omega_4^- \\
\nabla \phi \cdot n = 0 \quad (x, y) \in \Omega_4^+$$

(7b)

\n
(7c)

(7d)

where $\nabla$ is the gradient operator, and $n$ is the unit normal vector. Equation (7a) arises from the symmetric nature of the present problem. Equations (7b) and (7c) imply that both the electric potential and the electric field are continuous across the membrane-liquid interface. Note that if the dielectric constant of the membrane layer $\varepsilon_1$ is different from that of the bulk liquid phase $\varepsilon_2$, then eq (2) should be modified accordingly, and a correction factor $\varepsilon = \varepsilon_1/\varepsilon_2$ needs to be added to the right-hand side of eq (7c). For simplicity, we assume $\varepsilon = 1$. Equation (7d) suggests that the electric field vanishes on the rigid core of microchannel. In terms of scaled symbols, eqs (7a)-(7d) become

$$\frac{\partial^2 \Phi}{\partial x^2} + \frac{\partial^2 \Phi}{\partial y^2} = K^2 (G + jN) \frac{1}{a+b} \quad \Omega \in \mathbb{Y}, \mathbb{X} \quad \Phi \Omega_4^+ = \Phi \Omega_4^- \\
\nabla \Phi \cdot n = 0 \quad (X, Y) \in \Omega_1, \Omega_3 \\
\Phi \Omega_4^+ = \Phi \Omega_4^- \\
\n(\mathbf{8a})$$

$$\Phi \Omega_4^+ = \Phi \Omega_4^-$$

$$\nabla \Phi \cdot n = 0 \quad (X, Y) \in \Omega_2$$

$$\nabla \Phi \cdot n = 0 \quad (X, Y) \in \Omega_2$$

(8b)

(8c)

(8d)

For incompressible fluid, $u(x,y)$ is described by the Navier-Stokes equation

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = -\left[-(\partial p/\partial z) + \rho_{el}E_z - ju\right] \quad \eta$$

(9)

where $\gamma$ is friction coefficient of membrane layer per unit volume. This expression can be rewritten in scaled form as

$$\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} = K^2 \left[ \frac{L - G}{a+b} + M + j\lambda^2 \right]$$

(10)

where $U = u/u_0$, $L = \varepsilon RT_{z} \eta F u_0$, $\lambda^2 = \gamma / \eta \kappa$, $M = P / \eta \kappa u_0$, $u_0$ is a reference velocity. The boundary conditions associated with eq (9) are assumed as

$$\nabla u \cdot n = 0 \quad (x, y) \in \Omega_1, \Omega_3$$

$$u \Omega_4^+ = u \Omega_4^-$$

(11a)

(11b)
\[ \nabla u \cdot n_{\Omega_1} = \nabla u \cdot n_{\Omega_4} \]  
\( u = 0, \ (x, y) \in \Omega_2 \) \hspace{1cm} (11d)

Equation (11a) arises from the symmetric nature of the system, and eqs (11b) and (11c) imply that both the velocity and the shear stress are continuous across the membrane-liquid interface. Note that if the viscosity of the liquid in the membrane phase \( \eta_1 \) is different from that of the bulk liquid phase \( \eta_2 \), eq (9) should be modified accordingly, and a correction factor \( \eta' = \eta_1 / \eta_2 \) should be added to the right-hand side of eq (11c). Under typical conditions, however, because the porosity of membrane is large, we assume that \( \eta_1 \approx \eta_2 \), and, therefore, \( \eta' \approx 1 \). Equation (11d) arises from the non-slip nature of rigid wall.

The volumetric flow rate arising from the electroosmosis can be evaluated by

\[ V_i = 4 \int_{\Omega} ud\Omega = 4 \int_0^H \left[ \int_0^L \left( 1 + \gamma^2 / H^2 \right)^{1/2} -1 \right] W^2 u(x, y) dx dy, \]  
P=0 \hspace{1cm} (13)

In terms of scaled symbols, we have

\[ V_i = 4D_h^2 u_0 \int_0^H \left[ \int_0^L \left( 1 + \gamma^2 / H^2 \right)^{1/2} -1 \right] H U(X, Y) dX dY \]  
(14)

四、結果與討論

The performance of the elliptical microchannel considered is examined through numerical simulation. The equations governing the electric field and flow field and the associated boundary conditions are solved by FlexPDE, a commercial software based on finite element method. For illustration, we assume that the liquid phase contains 1:1 electrolyte, and the membrane layer is negatively charged with \( w=-1 \). The value of \( \gamma \) is estimated by modified Rouse theory, and for polydimethylsiloxane, which predicts that \( \gamma = 10^{13} \) (N \( \cdot \) s/m\(^4\)). According to Mala et al., if the bulk concentration of electrolyte is in the range 10\(^{-4}\) to 10\(^{-6}\) M, then the zeta potential ranges from 100 to 200 mV. Therefore, the amount of fixed charge per unit length of membrane layer is assumed the value of 10\(^{-7}\) C/m, which yields an appropriate surface potential. Also, we assume \( f_a = f_i = 10^{-12} \) kg/s, \( T = 298 \) K, \( \varepsilon = 7.08 \times 10^{-10} \) C/(V \( \cdot \) m), \( \eta = 9 \times 10^{-4} \) kg/(m \( \cdot \) s), and \( u_0 = 10^{-3} \) m/s.

For a fixed \( H/W \), the thinner the membrane layer, the higher the \( |\Phi| \), and for a fixed membrane thickness, the smaller the \( H/W \), the higher the \( \Phi \). For a fixed \( d \), the smaller the \( H/W \), the smaller the magnitude of the liquid velocity at the center of the microchannel. This is because if \( D_h \) is fixed, the smaller the \( H/W \) the narrower the fluid flow through the membrane layer, the more significant the non-slip effect of channel wall, and therefore, the slower the velocity of fluid. For a fixed \( H/W \), the thinner the membrane layer the greater the magnitude of the liquid velocity at the center of the microchannel.

五、參考文獻