Numerical Simulation on Electro-Osmotic-Flow in Microchannel

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Abstract - *The drive mode of fluid body in microchannel is a key in microfluidic control system. Electro-Osmotic MicroPump (EOP) is a microfluidic system which is controlled by electric field with no moving parts. EOPs are attracting increasing attention due to the ease of fluid control in complex microchannels. The theory of forming Electro-Osmotic-Flow (EOF) is analyzed and governing equations are given based on the mechanism forming EOF. After analyzing and simplifying governing equations, numerical simulation of those equations is performed by finite difference method and vorticity-stream function. Simulation results interpret the relations between parameters, which offer the foundation to research EOP.*
Keywords: Electro-osmotic-flow, Double electro layer, Numerical simulation

1 Intraduction

Within the rapidly growing realm of microelectromechanical systems (MEMS), biological systems such as micro-total analysis systems (μTAS) have received much attention in recent years [1-4]. Samples can be analyzed in much less time, much less wasted material and much less pollution using these micro-channel based devices. It is a key technology of micro flux drive and control. Many micropumps are investigated in the latest years, but their drive and control technologies still remain challenge.

There are two types of micropumps: mechanical and non-mechanical. It is recognized non-mechanical micropumps are better than mechanical ones. Electro osmotic flow micropump (EOFP) is one type of nonmechanical micropumps. EOFP is simple and effective, --electrodynamic force acts on theliquid directly and microchannel on the microchip is the main part of micropump. So EOFP has simple structure and non active mechanical parts, no valve and no mechanical parts. The flow field in EOFP is uniform and the concentration of bio-sample or chemical sample is diffused less flowing in microchannel, which is useful to transport and separate sample. That is why EOFP can find wide applications , such as drug delivery system, non-needle injector, bio-chemical synthesize and analysis, DNS and protein analysis, and etc. [5, 6]

2 The mechanism of electroosmotic flow

2.1 Electroosmotic flow

Generally, there are charges on most interface between solid and liquid, that is, when electrolyte contracts the surface of solid, the solid surface will produce charges for ionization , ion adsorption and ion dissolve, and other complex chemistry, At the same time, those surface charges influence on the ion distribution in electrolyte, which forms EDL[7]. EDL has two parts: one is the negative ion layer inside micro channel wall, and the other is the positive ion layer on the wall, this layer named Stern layer. There is a layer outside Stern layer named diffuse layer. The potential on Stern layer named zeta potential.

For example, the material of micro channel is silicon, the fluid in micro channel is alkalescence, which ionizes the free hydroxyl groups of silicon ($SiOH \leftrightarrow SiO^{-} + H^{+}$). SiO^{-} concentrates highly in the micro channel forming the negative ion layer, then it absorbs the cations in electrolyte forming Stern layer. When an electric field E is acted on the ends of the micro channel, the cations in electrolyte are moved directionally forming EOF with molecules surrounding them. The principle of EOF is shown in figure 1. Generally, Stern layer doesn't move for absorption, we called the plane as plane of shear. Outside the diffuse layer, there is a surface above which EOF velocity doesn't change, this surface is named plane of slip.

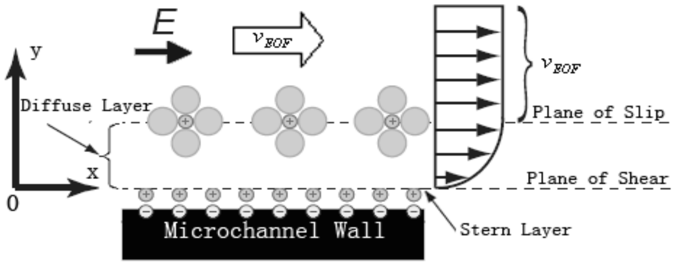


Fig.1 *EOF Forming Mechanism*

2.2 EDL mathematic model

Based on the electrostatic, the relation between zeta potential and charge density in electrolyte satisfies the Poisson equation at any point in electrolyte [8].

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} = -\frac{\rho_e}{\varepsilon \varepsilon_e} \quad (1)$$

where ε is dielectric constant; ε_e is permittivity of vacuum; ρ_e is the net charge density.

When a system is under the state of thermal equilibrium, the ions in electrolyte satisfy Boltamann distribution:

$$n_i = n_{i0} \exp(-\frac{z_i e \psi}{K_b T}) \quad （2）$$

where n_i is concentration of type i ion; n_{i0} is bulk ionic concentration of type i ion; z_i is electrovalence of type i ion; e is the charge of a proton; Kb is Boltamann constant; T is absolute temperature.

The net charge density can be expressed:

$$\rho_e = e \sum_{i=1}^{N} z_i n_{i0} \exp(-\frac{z_i e \psi}{K_b T}) \quad (3)$$

where N is the number of the ion types.

To solve the equation (1), the following dimensionless parameters are defined: $x^* = \frac{x}{W}$, $y^* = \frac{y}{W}$, $\psi^* = \frac{ze\psi}{K_b T}$, where W is the characteristic width of microchannel. Substitute them into equation (1）:

$$\frac{\partial^2 \psi^*}{\partial x^{*2}} + \frac{\partial^2 \psi^*}{\partial y^{*2}} = \frac{2W^2 z^2 e^2 n_0}{K_b T \varepsilon \varepsilon_0} \sinh(\psi^*) \quad （4）$$

Set $L_D^{-1} = (\frac{2n_0 e^2 z^2}{K_b T \varepsilon\varepsilon_0})^{\frac{1}{2}}$, it is called Debye parameter, so equation (4) can be written:

$$\frac{\partial^2 \psi^*}{\partial x^{*2}} + \frac{\partial^2 \psi^*}{\partial y^{*2}} = \frac{W^2}{L_D^2}\sinh(\psi^*) \qquad (5)$$

3 EOF governing equations

The phenomenon in microchannel flow can't be explained for electrokinetic effects and the influence of EDL. So it is a key to embody the EDL influence when use the method of numerical simulation to describe microflow.

3.1 The potential ϕ caused by the electric field *E*

The distribution of the electric field potential ϕ in microchannel satisfies Laplace equation [7]:

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = 0 \qquad (6)$$

Define the dimensionless parameters $x^* = \frac{x}{W}$, $y^* = \frac{y}{W}$, $\phi^* = \frac{\phi}{\phi_1}$, substitute them into equation (6):

$$\frac{\partial^2 \phi^*}{\partial x^{*2}} + \frac{\partial^2 \phi^*}{\partial y^{*2}} = 0 \qquad (7)$$

3.2 EOF flow field

Electrically driven force acted on the flow in microchannel is caused by the interaction of electric field and charge, so the force can be expressed: $\vec{F} = \rho_e \vec{E}$ where $\vec{E} = -\nabla(\phi + \psi)$.

Flow continuity equation in microchannel:

$$\nabla \vec{V} = 0 \qquad (8)$$

Navier-Stokes equation[9] described the EOF flow field after adding force correction term can be written:

$$\rho\left[\frac{\partial \vec{V}}{\partial t} + \left(\vec{V}\cdot\nabla\right)\vec{V}\right] = -\nabla P + \mu\nabla^2\vec{V} + 2ezn_0\sinh(\frac{ze\psi}{K_b T})\cdot\nabla(\phi+\psi)\backslash \qquad (9)$$

where $\vec{V}$ is EOF velocity; P is pressure; ρ is the density of electrolyte; μ is the electrolyte viscosity.

Define the dimensionless parameters $t^* = \frac{tV}{L}$, $\overrightarrow{V^*} = \frac{\vec{V}}{V}$, $P^* = \frac{P}{\rho V^2}$, $y^* = \frac{y}{W}$, $\phi^* = \frac{ze\phi}{K_b T}$, $\psi^* = \frac{ze\psi}{K_b T}$, $x^* = \frac{x}{W}$, where $V = \sqrt{\frac{2n_0 k_b T}{\rho}}$. Substitute them into equations (8) and (9):

$$\nabla \overrightarrow{V^*} = 0 \tag{10}$$

$$\frac{\partial \overrightarrow{V^*}}{\partial t^*} + \left(\overrightarrow{V^*} \cdot \nabla\right)\overrightarrow{V^*} = -\frac{1}{\rho}\nabla P^* + \frac{1}{R_e}\nabla^2 \overrightarrow{V^*} + \sinh(\psi^*)\cdot \nabla(\phi^* + \psi^*) \tag{11}$$

where Re is Reynolds number, $\mathrm{Re} = \frac{\rho v_{EOF} W}{\eta}$.

The following will omitted the dimensionless symbol * for solving equations expediently.

4 Method solving EOF flow field equation

4.1 Equations of Poisson-Boltzmann and Laplace

About Poisson-Boltzmann equation, 2D microchannel and coordinates are shown as figure 2, when electrolyte filled in microchannel, its boundary conditions are:

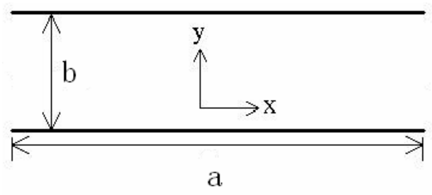


Fig.2 2D *Microchannel*

Inlet: $\frac{\partial \psi}{\partial y} = 0$ (x=0) ; Outlet: $\frac{\partial \psi}{\partial y} = 0$ (x=a) ; wall: $\psi = \zeta$ (y=0 and y=b)

The boundary conditions about Laplace equation are: $\phi = 0(x = 0)$, $\phi = E(x = a)$, $\frac{\partial \phi}{\partial x} = 0(y = 0, y = b)$.

Above two equations can employ finite difference method to solve after meshing uniformly [10].

4.2 Navier-Stokes equation

The difficult solving equation (11) is there is a pressure gradient in it, so the method of fluxion is employed. The velocity $\vec{V} = \begin{pmatrix} u \\ v \end{pmatrix}$ can be expressed with scalar field f in 2D microchannel.

Set $\nabla^{\perp} = (-\frac{\partial}{\partial y}, \frac{\partial}{\partial x})'$ 、 $u = -\frac{\partial f}{\partial y}$ 、 $v = \frac{\partial f}{\partial x}$, that is $\vec{V} = \nabla^{\perp} f$. Scalar field f is called fluxion function [11]. Then equation (10) can be expressed:

$$\nabla \vec{V} = (\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}) = (-\frac{\partial^2}{\partial x \partial y} + \frac{\partial^2}{\partial x \partial y}) f = 0 \tag{12}$$

Define $\omega = \nabla^{\perp} \vec{V}$, that is $\omega = \nabla^{\perp^2} f$, where ω is called vorticity. Equation (11) can be expressed:

$$\nabla^{\perp}[\frac{\partial\overline{V}}{\partial t}+\left(\overline{V}\cdot\nabla\right)\overline{V}]=\nabla^{\perp}[-\frac{1}{\rho}\nabla P+\frac{1}{R_e}\nabla^2\overline{V}+\sinh(\psi)\cdot\nabla(\phi+\psi)] \tag{13}$$

For $\nabla^{\perp}\nabla P=0$, so above equation can be written:

$$\frac{\partial\overline{\omega}}{\partial t}+\left(\overline{V}\cdot\nabla\right)\overline{\omega}=\frac{1}{R_e}(\nabla^2\overline{\omega})+\nabla^{\perp}\sinh(\psi)\cdot\nabla(\phi+\psi) \tag{14}$$

In electro osmotic drive the potential caused by electric field is much bigger than zeta potential, so in the expression $\nabla(\phi+\psi)$ can omitted ψ and vorticity doesn't change by time.

Based on the above discussion, equation (14) with boundary conditongs can be written:

$$\begin{cases}\left(\overline{V}\cdot\nabla\right)\overline{\omega}=\frac{1}{R_e}(\nabla^2\overline{\omega})+\nabla^{\perp}\sinh(\psi)\cdot\nabla\phi \\ \overline{\omega}=\nabla^{\perp^2}f \\ \overline{V}=\nabla^{\perp}f \\ f\mid_{\partial D}=0 \\ \frac{\partial f}{\partial n}\mid_{\partial D}=0\end{cases} \tag{15}$$

This equations simplify solving Navier-Stokes equation.

5 Simulation conclusions and discuss

Before simulating, assume parameters: $\varepsilon=80$, $\varepsilon_e=8.854\times10^{-12}c^2/nm^2$, $n_{i0}=6.022\times10^{19}m^{-3}$, $e=1.6\times10^{-19}C$, $K_b=1.38\times10^{-23}JK^{-1}$, $T=300K$.

With parameters and equation (15), zeta potential, electric field potential and EOF velocity can be simulated based on difference method.

Isopotential of zeta potential in 2D microchannel is shown as figure 3. Form figure 3 it is shown that the gradient of zeta potential is 0 along x direction. Figure 4 shows the value of zeta potential from the wall to the center of microchannel is decreased by exponent law.

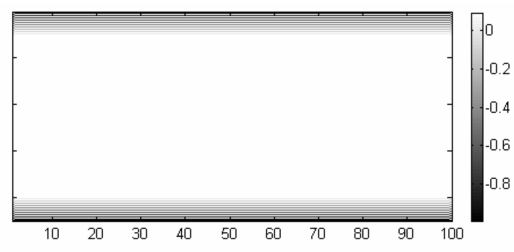


Fig.3 *Isopotential of zeta potential*

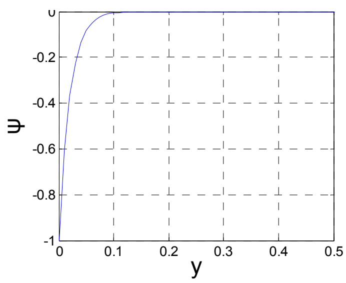
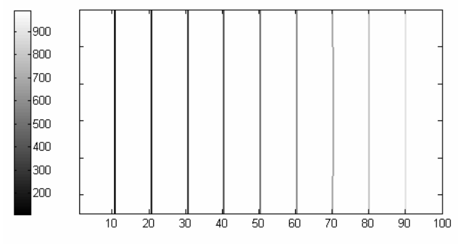
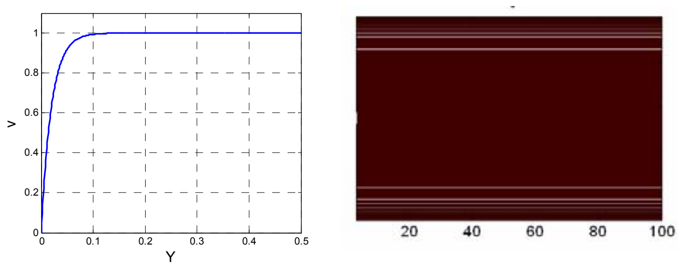


Fig.4 *Distribution of zeta potential along y*

The potential of electric field distribution is shown as figure 5(E=1000v/cm), from figure 5, it is shown the electric field is uniform.





a) EOF velocity distribution along y   b) EOF velocity distribution along x

Fig 5. *The distribution of electric field*   Fig. 6 *EOF velocity distribution*

EOF velocity distribution is shown as figure 6. From figure 6, the gradient of velocity along x direction is 0 and along y direction vary by exponent.

6 Conclusion

Numerical simulation of the microflow in microchannel is given in this paper based on EOF mechanism. The dimensionless equations of zeta potential and electric field potential are given by analysis. The control equation is simplified by use of fluxion function. Simulation conclusions show:

1. The gradient of zeta potential is 0 along x direction, that is the direction along the microchannel wall;
2. The distribution of electric field is uniform;
3. The EOF volecity away from the wall is equal, the figure of EOF volecity like as plug.
4. All above conclusions are the theory base for microfluidic control in designing micropump.

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8 References

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