Numerical Simulation of Seawater Desalination Effect in The Micro-Nanochannel

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Abstract. In recent years, the study on the micro-nanochannel in the microfluidic technology has been made significant progress for which when inner walls charged can function similarly as ion permselective membrane. This article constructed one symmetric model with three parallel microchannels connected with two sets of nanochannel arrays and explained the mechanism of desalination within the channel by using numerical simulation method. For example, when the voltage difference, $V_{cn}$, across the nanochannel array is equal to $10V_T$, the desalting efficiency can have reached nearly 90%; as the $V_{cn}$ is increased continuously to $20V_T$, the desalination rate will definitely exceed 99% and as the $V_{cn}$ increases the rate increases more slowly.

1. Introduction

People have done much study on electroosmosis since the phenomenon of which was revealed by Reuss for the first time in 1809 [1]. For almost materials, when they are contacted with the electrolyte solution, there will be bulk of negative charge accumulating at the interface of matter and solution and these charges will affect the distribution of other particles or ions. Generally, the co-ions will get away from the surface of the matter due to the rejection, yet the counter ions are attracted to the vicinity of the interface, forming a diffusion layer that the ion concentration of which varied gradually from the surface to the outer space, this phenomenon is called ICP (ion concentration polarization) [2-4]. When the surface is under a parallel tangential electric field, the particles in the solution will be powered by the electric field force and move with the solution together in one specific direction, namely the electroosmosis mentioned above. It has been proved that the nanochannel has the same function of the ion permselective membrane, namely just allowing one kind of charged specie to pass through. Kim [5] used the micro-nanochannel to design two kinds of seawater desalination systems, H-shaped, based on ICP. Han [6] developed another Y-shaped structure also using ICP to reach the same goal. Besides, H-shaped structure can also be used to do the enrichment or separation of charged particles in chemistry. This article mainly did the simulation of the sea water desalting effect in the micro-nanochannel based on ICP, with the help of nanochannel array’s ion permselective function.

2. System setup

As is shown in Fig. 1, this model is mainly consisted of one central and two parallel microchannels connected by two sets of nanochannel arrays. In the photo, the length and height of central microchannel are $L_2=20\mu m$ and $H_1=2\mu m$, respectively. The nanochannel array contains 9 nanochannels, positioning
the center of two sides of the central microchannel and the sizes of which are height \( h_1 = 1\mu m \) and 1nm's width. The parallel microchannel is a rectangle of length \( L_3 = 10\mu m \) and height \( h_2 = 1\mu m \). Lastly, the central microchannel is connected by two buffer reservoirs of which the sizes are length \( L_1 = 10\mu m \) and height \( H_2 = 20\mu m \), respectively. The inner walls of the whole system are all negatively charged with the surface charge density of \( \sigma = -5.5mC/m^2 \) except the buffer reservoir. At first, all the channels are filled with KCL electrolyte solution, the concentration of which is \( C_0 = 1mM \). The diffusion coefficient of \( K^+ \) and \( Cl^- \) are \( D_+ = 1.957 \times 10^{-9}m^2/s \) and \( D_- = 2.032 \times 10^{-9}m^2/s \), respectively. Besides, we apply two different voltages \( V_L \) and \( V_R (V_L > V_R) \) to the two sides of the two reservoirs to generate a tangential electric field along the central microchannel. The voltages to the four outlets of the two parallel microchannels are all set to \( V_g = 0 \), namely connected to the ground. We define \( V_{LR} = V_L - V_R \) as the potential drop between the inlet and outlet of the central channel and set the pressures at the boundary of which are all equal to 0 to guarantee the fluid motion is strictly powered by the electric force. For convenience, a term cross nanochannel voltage \( V_{cn} = (V_L + V_R) - V_g \) is defined as the difference between voltage at the nanochannel array location determined by external electric field without ICP and the actual voltage applied at the nanochannel array, representing the voltage drop across the microchannel/array junction in actual experiments. In this equation, the bigger \( V_g \) corresponds to the smaller \( V_{cn} \) and weaker ion concentration polarization.

![Fig. 1 Schematic sketch of ICP system.](image)

3. Governing equations and corresponding boundary conditions

The governing equations for incompressible fluid flow, transport of ions, and electric potential are the Navier-Stokes, Nernst-Plank, and Poisson equations [7], respectively,

\[
\rho \left( \frac{\partial \mathbf{U}}{\partial t} + (\mathbf{U} \cdot \nabla) \mathbf{U} \right) = -\nabla P + \eta \nabla \cdot \mathbf{U} + \rho_e E. 
\]

(1)

\[
\nabla \cdot \mathbf{U} = 0. 
\]

(2)

\[
\frac{\partial C_\pm}{\partial t} = -\nabla \cdot \mathbf{J}_\pm. 
\]

(3)

\[
\mathbf{J}_\pm = -\left( D_\pm \nabla C_\pm + Z_\pm \left( \frac{D_\pm F}{RT} \right) C_\pm \nabla \Phi \right) + \mathbf{U} C_\pm. 
\]

(4)

\[
-\nabla \cdot (\varepsilon \nabla \Phi) = \rho_e. 
\]

(5)

Here, \( \mathbf{U} \) is the velocity of the fluid, \( P \) is the pressure, and \( \Phi \) is the electric potential. We assume \( C_\pm \equiv C_\pm (x,y,t) \) and \( C \equiv C (x,y,t) \) represent the concentration of species at the location of \((x, y)\) and time \( t \). Constants \( \rho \) and \( \eta \) are the mass density and dynamic viscosity of the solution, respectively. The last
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An item $\rho E$ in equation (1) represents the force that electric field has on the unit volume solution. In the equations (3) and (4), constants $F$ and $R$ are Faraday's constant and gas constant, respectively. $T=300K$ is the temperature. $D_\pm$, $Z_\pm$ and $J_\pm$ are diffusion coefficients, valences and flux density of the species in the solution.

The boundary conditions of this system are as follows [5, 8]:

At reservoirs walls the boundary conditions are: (1) no-slip condition for fluid velocity; (2) constant surface charge density; (3) impermeable to all anions and cations:

$$U=0, \sigma=-5.5\text{mC/m}^2, J_+\cdot n=0, J_-\cdot n=0.$$  \hspace{1cm} (6)

where $n$ is the normal vector perpendicular to the boundary pointing out of the fluid domain. At the inlet boundary: (1) concentration of all ions are the same as those in the inlet reservoir; (2) the electric potential is $V_L$; (3) the pressure is 0.

$$C_+=C_0, C_-=C_0, \Phi=V_L, \nabla U\cdot n=0, P=0.$$  \hspace{1cm} (7)

At outlet boundary: (1) the electric potential is $V_R$; (2) free boundary conditions are applied for fluid flow; (3) the pressure is 0.

$$\Phi=V_R, \nabla U\cdot n=0, \nabla C_+\cdot n=0, \nabla C_-\cdot n=0, P=0.$$  \hspace{1cm} (8)

At the four boundaries of two parallel microchannels: (1) the concentration of the solution is $C_0$; (2) the electric potential is $V_G$; (3) the pressure is 0.

4. Results and discussion

When the $V_{cn}$ is equal to 0, there is no ICP phenomenon in the system. The overall concentrations of the cation and anion in the channel are both $C_0$ except the area of the nanochannel array and the main motion of fluid is EOF1 (electroosmosis of the first kind). When the concentration of the electrolyte solution is 1mM, the corresponding Debye Length of EDL (electric double layer) is 10nm. The width of nanochannel is 10nm, so the EDL will overlap in the nanochannel, namely only permitting the cation to pass through. As the value of $V_{cn}$ is increased continuously, there will be obvious voltage difference across the nanochannel array, so the cation can be powered to pass through the nanochannel and accumulate at the junction of nanochannel and parallel microchannel, while the anion will accumulate at the upper stream of the central microchannel due to the rejection. So, it can be observed that there will be a small area of low concentration electrolyte occurring at the vicinity of nanochannel which will extend towards the downer stream of microchannel as the fluid flows continuously. When the $V_{cn}$ is increased to 20 $V_T$ (thermal voltage, 25.8mV), the solution in the downer stream will only contain a very little electrolyte.

As is shown in the Fig. 2, for the model is symmetric, so we just give the half of the result. It shows the distribution of the concentration of anion in the system with $V_L=25V_T$, $V_R=0$ and $V_{cn}=15V_T$. In this situation, we can get the average concentration of the anion at the outlet is about 0.034mM and the desalination efficiency can be reached about 96.6%.

Fig. 2 Distribution of the concentration of anion in the channel at VLR=25VT and Vcn=15VT.
To explain the desalination effect more conveniently, we show the following results neglecting the reservoirs. Fig. 3 shows the dependence of the average concentration of cation along the center line of different values of $V_{cn}$ at the condition of $V_{LR}=25V_T$ and Fig. 4 gives out the curve of variation tendency of the concentration of cation at the outlet. From the two pictures, we can conclude that when the fluid flows to the vicinity of the nanochannel array along the $x$-axis, the concentration of the cation starts to decline and stay at a relatively low level in the downstream of the channel. When the $V_{cn}$ is equal to $10V_T$, the system's desalination efficiency can reach 90%. From Fig. 4, we can clearly see that when the $V_{cn}$ is increased to $20V_T$, the desalting rate can exceed 99% finally and as the $V_{cn}$ becomes bigger, the efficiency increases more slowly.

![Fig. 3 Distribution of the concentration of cation along the symmetric axis line at different values of $V_{cn}$ and $V_{LR}=25V_T$ (grey wireframe indicates the position of nanochannel array).](image1)

![Fig. 4 The average concentration of cation at the outlet at different values of $V_{cn}$ and $V_{LR}=25V_T$.](image2)

5. Conclusion

In this paper, the numerical simulation model is built up to compute the concentration field of anion in the microchannel and explain the mechanism of desalination effect based on ICP. Via the simulation, we can get the conclusion that the voltage difference $V_{cn}$ across the nanochannel array plays an important role in the desalination. While the $V_{cn}$ is at a low level, the system has gotten an effective result in desalination; when we continue to improve the value of $V_{cn}$ to $20V_T$, the efficiency can rise up to nearly 99%.
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