

# Modeling of Electro-osmotic Flow and Particle Transport in Micro-/Nanozzles

Electro-osmotic flow in micro-/nanozzles is important in many applications, such as electrical measurements on living cells and the injection and manipulation of DNA fragments into living cells. Understanding the theory behind transport of particles in micro-/nanochannels is essential to efficient design of any micro-/nanofluidic device.

## Calculation of the imposed electric field

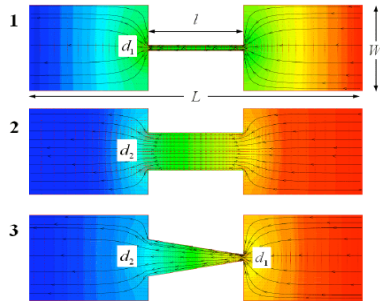
We have calculated the electric field for the reservoir-nozzle system. The geometry of the reservoir and nozzle/channel systems is shown in Figure 1, and three configurations are calculated. The imposed electric field satisfies Maxwell's equation

$$\nabla \cdot \overline{E}_i^* = 0 \Rightarrow E_i^*(x)A^*(x) = \text{constant}$$

Usually in experiments the potential drop is given and this potential drop can be written as

$$\Delta\phi_i^* = \phi_i^*(L) - \phi_i^*(0) = -\int_0^L E_i^*(x_0) dx = -E_i^*(x_0) \int_0^L \frac{A^*(x_0)}{A^*(x)} dx$$

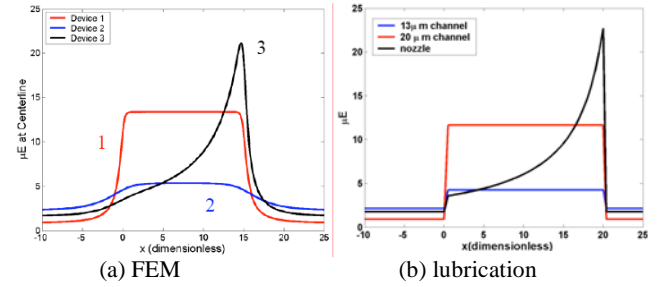
where  $E_i^*(0)$  and  $A^*(0)$  are the magnitude of the imposed electric field and cross-sectional area at a reference point  $x = x_0$ , and usually the inlet of the channel/nozzle is chosen as  $x_0$ . For a straight channel, away from the inlet and outlet regions, the imposed electric field is a constant. For a nozzle/diffuser, based on the lubrication theory, the dimensionless imposed electric field is  $E_x^i = 1/h$ , where  $h$  is the dimensionless half height of the nozzle/diffuser.



**Figure 1.** The calculated applied field for the reservoir and channel/nozzle system by Hu's group. The parameters are given by  $L = 105d_1$ ,  $l = 15d_1$ ,  $W = 15d_1$ ,  $d_2 = 6.5d_1$ .

Xin Hu has investigated three reservoir-nozzle or channel systems, as shown in Figure 1. The third case is a nozzle connected to two reservoirs, which is used in the experiments. The other two cases are channels having the same width as the large and small ends of the nozzle, respectively. The imposed electric field in  $x$  direction is compared for these three different cases in Figure 2. It is shown

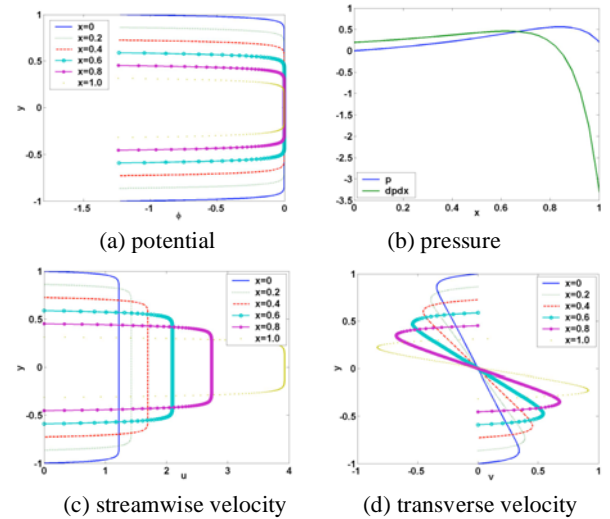
that the highest electric field is obtained for the nozzle case, and it is located at the sharp end of the nozzle. The lubrication results are shown on the right and are qualitatively similar to Hu's results (on the left), which are based on the finite element methods (FEM).



**Figure 2.** The imposed electric field calculated from (a) FEM and (b) lubrication theory.

## Nonlinear EOF

The previously analytical solution is obtained for the electro-osmotic flow in nanozzles/diffusers based on the Debye-Huckel approximation, which is accurate only for low potential ( $\phi \ll 26\text{mV}$ ). We have extended the calculation to a high potential field using the Poisson-Boltzmann distribution for ionic species. The electrical potential due to the presence of electric double layers (EDLs) is calculated numerically based on the Poisson-Boltzmann equation in the lubrication limit. The velocity field is calculated numerically using coordinates transformed by  $\eta = y/h$ ,  $\xi = x$ , which transforms the nozzle geometry into a rectangular geometry for easier to discretization of the equations. The Thomas algorithm is used to solve the potential and pressure equations.

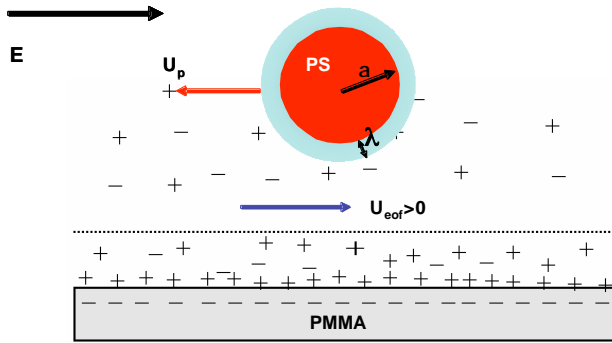


**Figure 3.** The potential, pressure and velocity field calculated for EOF in the nanozzle used by Singer's group for MD simulation. The surface charge density is  $-0.07 \text{ C/m}^2$ , and the solution is  $0.8\text{M NaCl}$ . The inlet is  $14.6 \text{ nm}$ , and the outlet is  $4.6 \text{ nm}$ . The length of the nozzle is  $15 \text{ nm}$ .

Based on this program, the results shown in Figure 3 are the results produced for Prof. Singer's group as an initial input for their molecular dynamic (MD) simulation. As shown in Figure 3, the dimensionless wall potential is in the order of 1 ( $\phi/26mV \sim O(1)$ ), which indicates the previous DH calculation will not be able to accurately predict the results for this case.

### Particle Transport

Xin Hu and Shengnian Wang have performed experiments to investigate the transport of the particles in microchannels. The particle velocity has been evaluated for the experimental parameters. Previously, the particles were evaluated as an ionic species in the solution, since the solution is de-ionized water, and the Debye length is large compared to the particle radius. Recently, the electrophoretic velocity of the particles was evaluated considering the effect of electrolyte solution.



**Figure 4.** A charged particle in an EOF flow field. For the experimental setup, the particles are Polystyrene (PS) beads and the walls are made of Polymethyl-methacrylate (PMMA).

The movement of a charged particle in an EOF flow field is shown in Figure 4. The EOF velocity for a thin EDL is given by

$$U_{eof} = -\frac{\zeta_w \epsilon_e E_x}{\mu}$$

and the electrophoretic velocity of the particle is given by

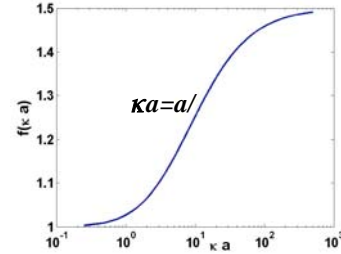
$$U_p - U_{eof} = \frac{2 \zeta_p \epsilon_e E_x}{3 \mu} f\left(\frac{a}{\lambda}\right)$$

The ratio of the velocity of the particle and the fluid flow is given by

$$\frac{U_p}{U_{eof}} = 1 - \frac{2 \zeta_p f\left(\frac{a}{\lambda}\right)}{3 \zeta_w}$$

where  $\zeta_p, \zeta_w$  are the zeta potential of the particles and the walls respectively and  $f$  is a function from Henry's solution for electrophoretic velocity. It is a function of the ratio of particle radius  $a$  to the Debye length  $\lambda$  and, as shown in Figure 5,  $f=1$  for small  $a/\lambda$  (thick EDLs) and  $f=1.5$  for large  $a/\lambda$  (thin EDLs). Since zeta potential is also affected by the concentration and the  $pH$  of the

solution, the ratio of  $U_p/U_{eof}$  depends strongly on the characteristics of the solution. Note that this ratio can be positive or negative depending on the zeta potentials of the particle and the wall. For different ionic solutions, the ratio of particle velocity and fluid velocity are evaluated in Table 1. The walls are made of PMMA, and the particles are 80 nm Polystyrene (PS) beads. For 0.1 M and 0.01 M solutions, the ratio of  $U_p/U_{eof}$  is positive, which means the particle is moving in the same direction as the fluid flow. For the last case, the ratio is negative, and it shows that the particles are moving in the opposite direction to the fluid flow. Note that the zeta potentials of PMMA and PS are obtained for  $pH=5.6$  solutions.



**Figure 5.** Henry's function  $f(a/\lambda)$ . In the limit of small  $a/\lambda$ ,  $f=1$ ; in the limit of large  $a/\lambda$ ,  $f=1.5$ .

C (M)	$\lambda$ (nm)	$\zeta_{PMMA}$ (mV)	$\zeta_{PS}$ (mV)	$f(\lambda/a)$	$U_p/U_{eof}$
0.1	1	-33	-40	1.4	0.23
0.01	3	-62	-70	1.29	0.23
0.001	10	-91	-50	1.13	-0.37

**Table 1.** Ratio of particle velocity to the fluid flow velocity for different solution concentration. The zeta potentials are obtained for  $pH=5.6$  solutions.

### Publications

1. L. Chen and A. T. Conlisk, Electroosmotic flow and particle transport in micro/nano nozzles and diffusers, *Biomedical Microdevices*, published online, December 2007, to appear 2008.
2. L. Chen and A. T. Conlisk, Electroosmotic flow micro/nano nozzles, AIAA paper 2007-0931, 45<sup>th</sup> Aerospace Sciences Meeting, Reno, Nevada, January 2007.
3. A. T. Conlisk, Ankan Kumar and Arfaan Rampersaud, Ionic and Biomolecular Transport in Nanochannels, *Nanoscale and Microscale Thermophysical Engineering*, **11**, nos. 1 and 2, pp. 177-199.
4. A. T. Conlisk, *Essentials of Micro and Nanofluidics with Applications in the Biological Sciences*, Cambridge University Press, 2009.
5. A. T. Conlisk, Book review, *Introduction to Microfluidics* by Patrick Tabeling, *J. Fluid Mech.*, **570**, pp. 503-505.