Poisson equation based modeling of DC and AC electroosmosis

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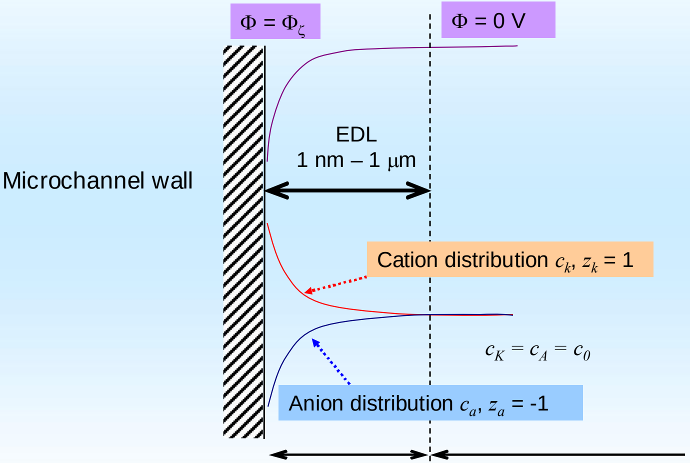
Electric double layer (EDL)



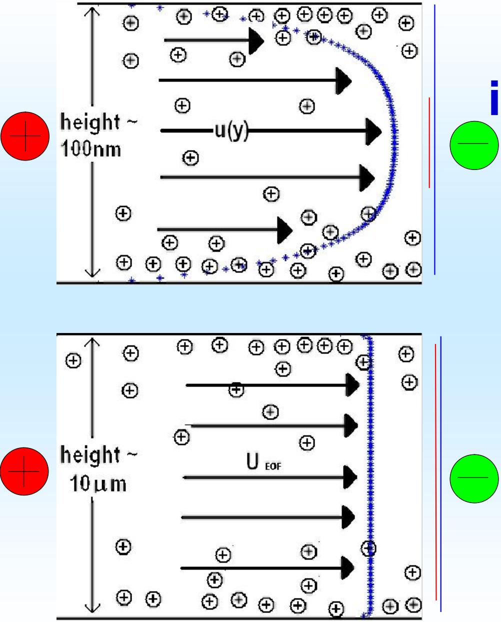
$$F\sum_i z_i c_i = q_{el} \neq 0$$

Non-zero electric charge

$$\sum_i z_i c_i = 0$$

Local electroneutrality

Electroosmosis induced by DC field



Positive ions accumulates at the charged surfaces

Axially imposed electric field acts on cloud of electric charge and starts fluid movement

nonslip

slip

Santiago J.G., Stanford microfluidic lab

Governing equations

- Mass balances of ionic components (at least 2 equations)

$$\frac{\partial c_i}{\partial t} = -\nabla \cdot \vec{J}_i + \sum_j \nu_{ij} r_j$$

- Navier-Stokes and continuity equations (3 or 4 equations, v_x, v_y, (v_z), p)

$$\rho \frac{D\vec{v}}{Dt} = \rho\vec{g} - \nabla P + \rho_{el}\vec{E} + \mu\nabla^2\vec{v}$$
$$\nabla \cdot \vec{v} = 0$$

- Poisson equation

$$\nabla \cdot \nabla\Phi = -\frac{\rho_{el}}{\varepsilon_0 \varepsilon_r}$$

Slip model of flow

- Simplified Navier-Stokes equation

$$\cancel{\rho\frac{D\vec{v}}{Dt}} = \cancel{\rho\vec{g}} - \nabla P + \cancel{\rho_{el}\vec{E}} + \mu\nabla^2\vec{v}$$

- Non-zero velocity on microcapillary walls (Helmholtz-Smoluchowski approximation)

$$\vec{v}\Big|_{wall} = -\mu_{eo}\vec{E}\Big|_{wall} \qquad \mu_{eo} = -\frac{\varepsilon_r\varepsilon_0\phi_\zeta}{\eta}$$

- Electroneutrality

$$\sum_i z_i c_i = 0 \;\Rightarrow\; \rho_{el} = 0 \;\Rightarrow\; \nabla\cdot\nabla\Phi = 0$$

Non-slip model of flow

- Navier-Stokes equation with electric volume force

$$\cancel{\rho \frac{D\vec{v}}{Dt}} = \cancel{\rho \vec{g}} - \nabla P + \rho_{el} \vec{E} + \mu \nabla^2 \vec{v}$$

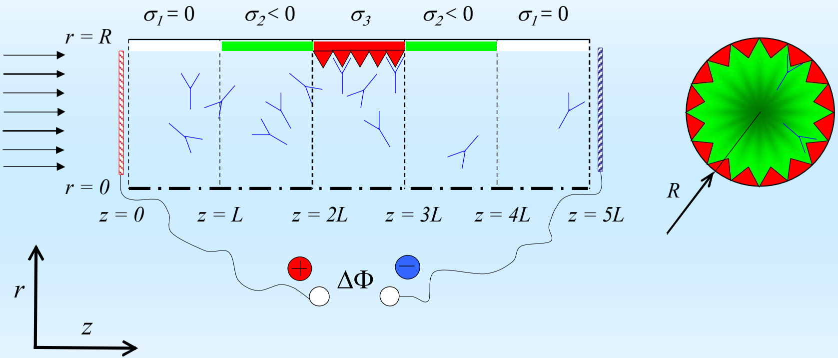
- Zero velocity

$$\vec{v}\Big|_{wall} = 0$$

- Local deviation from electroneutrality

$$\sum_i z_i c_i \neq 0 \;\Rightarrow\; \rho_{el} \neq 0 \;\Rightarrow\; \nabla \cdot \nabla \Phi = -\frac{\rho_{el}}{\varepsilon_0 \varepsilon_r}$$

Model of a biosenzor driven by an external DC electric field

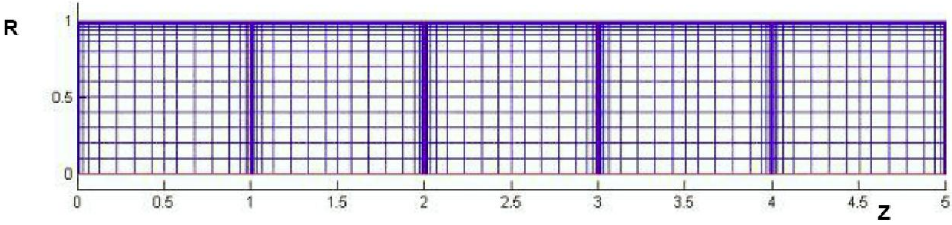


Ligand + Receptor = Complex
solution solid ph. solid ph.

Device consists of 5 compartments
DC electric field is applied
Electric charge attached to walls

Meshing

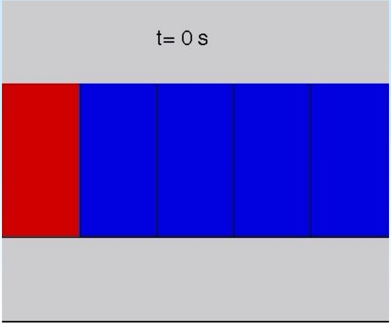
- 2860 rectangular elements
- non-equidistant
- anisotropic
- the ratio of the larger and the smaller edge of rectangles in interval 10^0 - 10^4



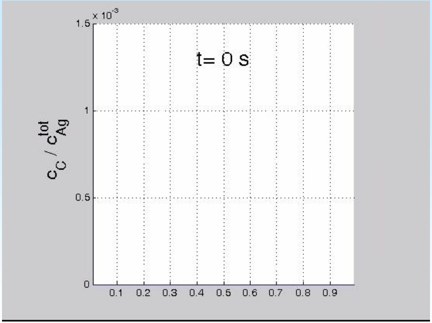
Short-time electrokinetic dosing of a ligand in aqueous solution

Formation of the ligand-receptor complex on microchannel wall

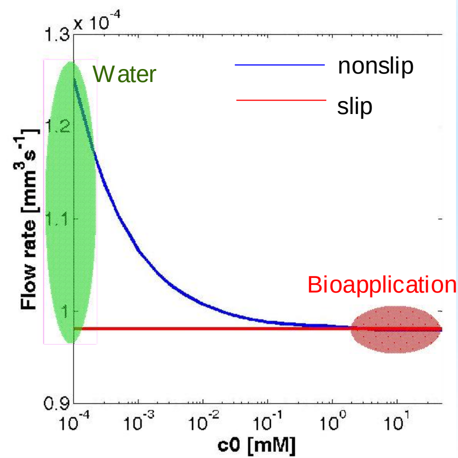
Ligand concentration field

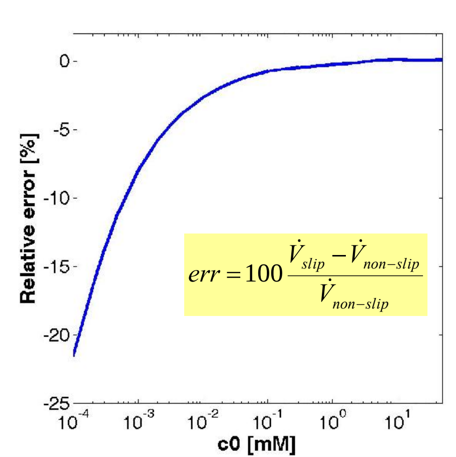


Level of saturation of the receptor binding sites



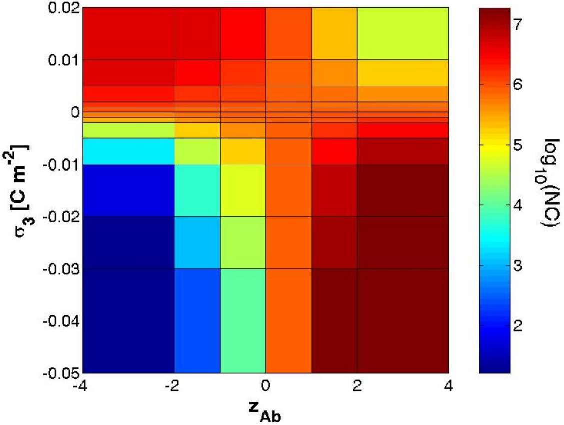
Example of limitation of the slip model – electrolyte concentration





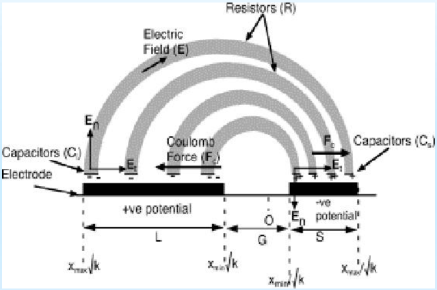
Example of the slip model limitations – ligand-wall (receptor) electrostatic interaction

Effects of the surface electric charge σ_3 and ligand charge number z_{Ab} on formation of ligand-receptor complex on the microchannel wall



NC is the total number of molecules of the ligand-receptor complex

Principle of AC electroosmosis



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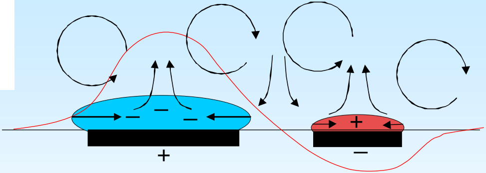
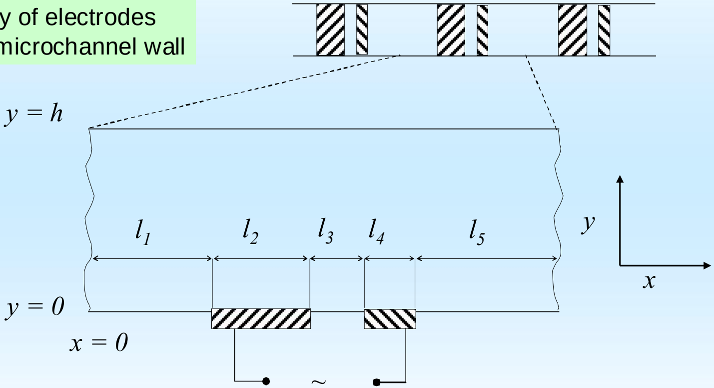


Distribution of electric potential along the electrodes (red line) induces tangential movement of the electric charge and thus eddies formation.

Model of electrokinetic flow driven by an AC electric field in a microchannel

Periodic array of electrodes deposited a microchannel wall

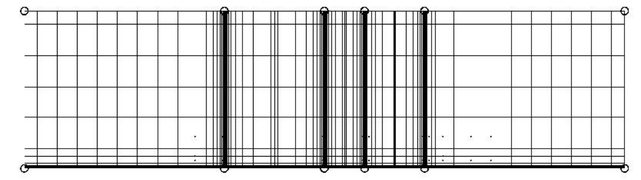


$$\Delta\Phi = A\sin(2\pi f t)$$

Geometry and dimensions of the microchannel
($l_1 = l_5 = h = 10$ μm, $l_2 = 5$ μm, $l_3 = 2$ μm, $l_4 = 3$ μm).

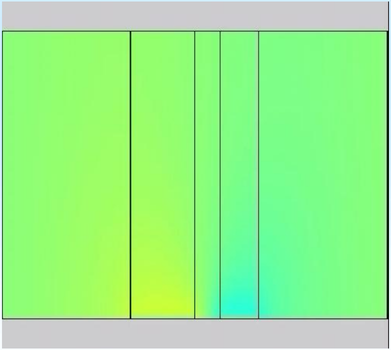
Meshing

- 2800 rectangular elements
- non-equidistant
- anisotropic
- the ratio of the larger and the smaller edge of rectangles in interval 10^0 - 2×10^4

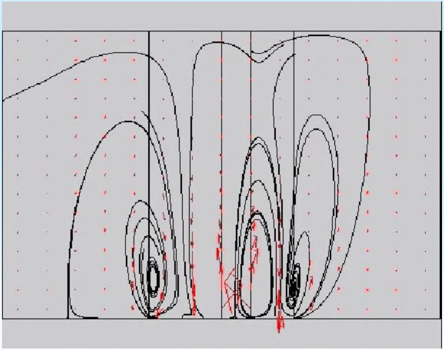


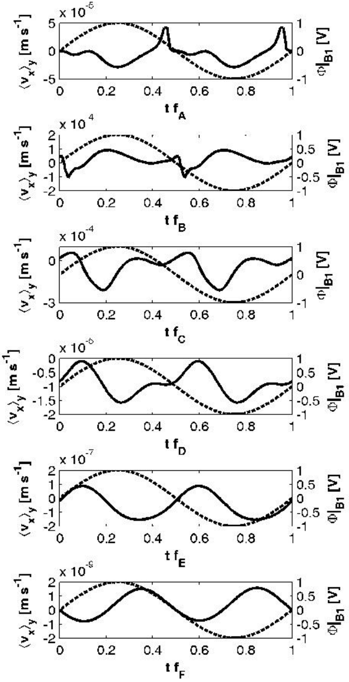
Steady periodic regime A = 1 V, f = 1 kHz

Electric potential distribution
(blue ΔΦ = -1V, red ΔΦ = +1V)



Velocity distribution





Time course of global velocity

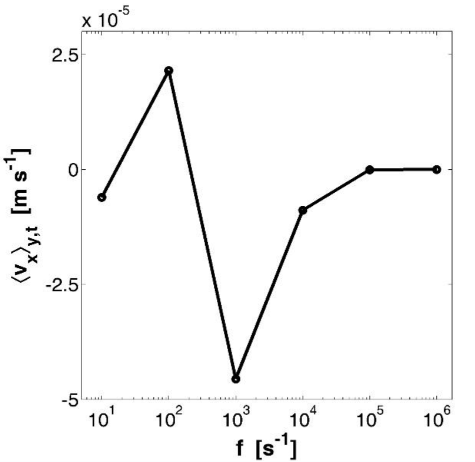
Global velocity = the tangential velocity v_x averaged over depth of the microchannel $y \in \langle 0\ ,\ h \rangle$

Most of the stable periodic regimes (except $f = 1\times10^4\ s^{-1}$) exhibits changes in flow direction during one period ($1/f$) $\Rightarrow$ fluid motion in the microchannel has a zigzag character.

However, a continuous flux of electrolyte can be experimentally observed because of high frequency of the zigzag motion ($2f$ or $4f$).

$f_A = 1\times10^1\ s^{-1}$, $f_B = 1\times10^2\ s^{-1}$, $f_C = 1\times10^3\ s^{-1}$,
$f_D = 1\times10^4\ s^{-1}$, $f_E = 1\times10^5\ s^{-1}$, $f_F = 1\times10^6\ s^{-1}$.

Dependence of global velocity on AC frequency, A = 1 V



The dependence of the global velocity averaged over one period ($1/f$) on the applied frequency of AC electric field.

This dependence is in a good qualitative agreement with the experimentally reported one. For the given set of parameters, there are several flow reversals observed in the studied frequency interval. The maximum global velocity is few tents of microns per secondd in the frequency interval $\langle 10^2, 10^4 \rangle$ Hz.

Conclusions

- COMSOL Multiphysics software enables numerical analysis of electro-transport processes based on EDL in macroscopic objects
- Slip approximation is not necessary
- Limitations of the slip approximation in a DC system were identified
- Electroosmosis induced by AC electric field was analyzed in a microfluidic channel
- Dependence of global velocity on AC frequency was computed
- Experimentally observed phenomenon (flow turnover at some frequencies) was proved by numerical analysis
- This phenomenon probably does not rely on chemical and/or electrode reaction