

Presented at the COMSOL Users Conference 2006 Prague

# Poisson equation based modeling of DC and AC electroosmosis

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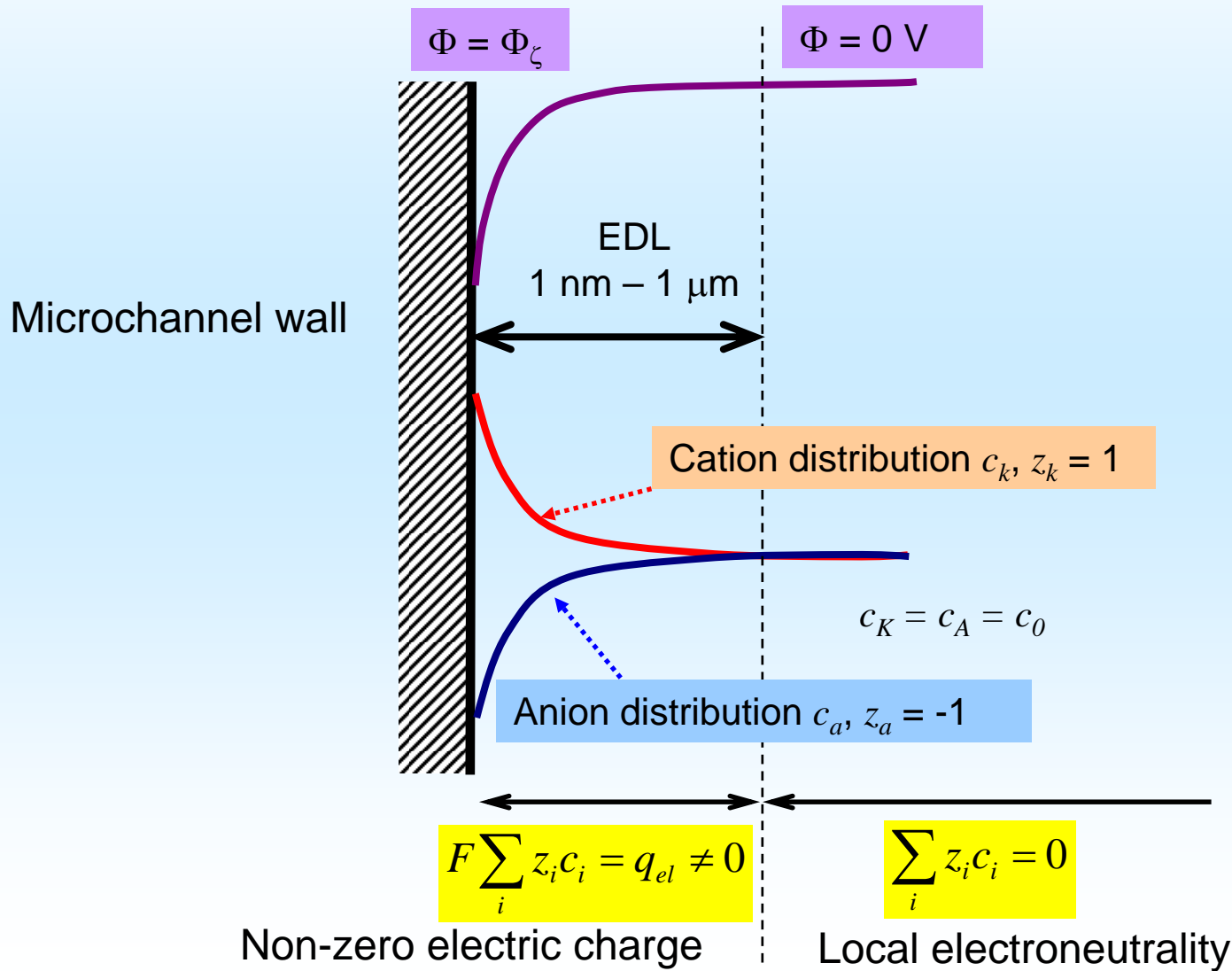
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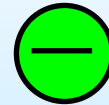
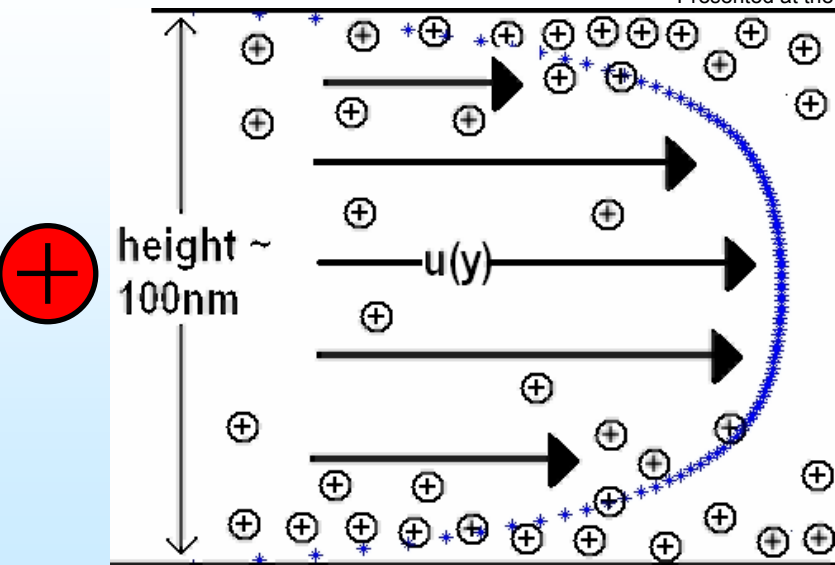
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# Electric double layer (EDL)



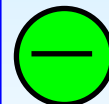
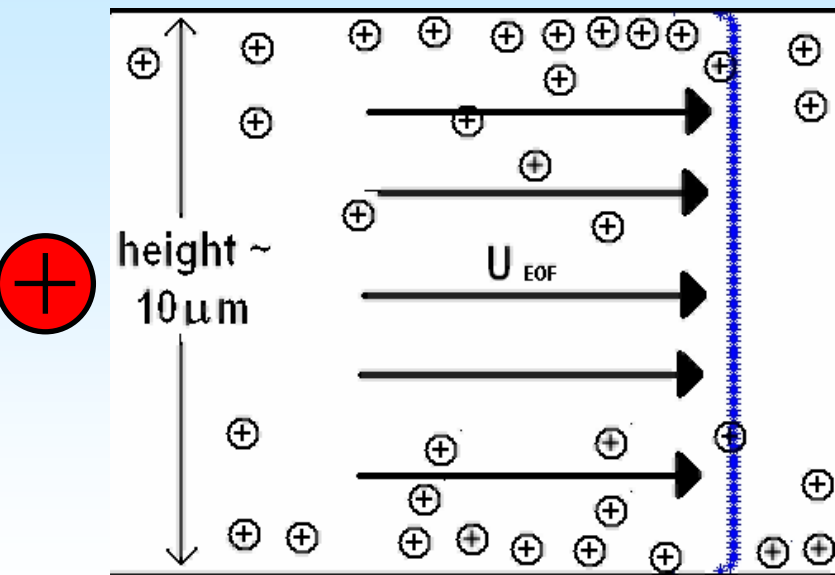
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# Electroosmosis induced by DC field

Positive ions accumulates at the charged surfaces

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



— nonslip  
— slip

# Governing equations

- Mass balances of ionic components (at least 2 equations)
- Navier-Stokes and continuity equations (3 or 4 equations,  $v_x$ ,  $v_y$ , ( $v_z$ ),  $p$ )
- Poisson equation

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

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

$$\nabla \cdot \nabla \Phi = -\frac{\rho_{el}}{\epsilon_0 \epsilon_r}$$

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# Slip model of flow

- Simplified Navier-Stokes equation

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

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

$$\vec{v}|_{wall} = -\mu_{eo} \vec{E}|_{wall} \quad \mu_{eo} = -\frac{\epsilon_r \epsilon_0 \phi_\zeta}{\eta}$$

- Electroneutrality

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

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# Non-slip model of flow

- Navier-Stokes equation with electric volume force

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

- Zero velocity

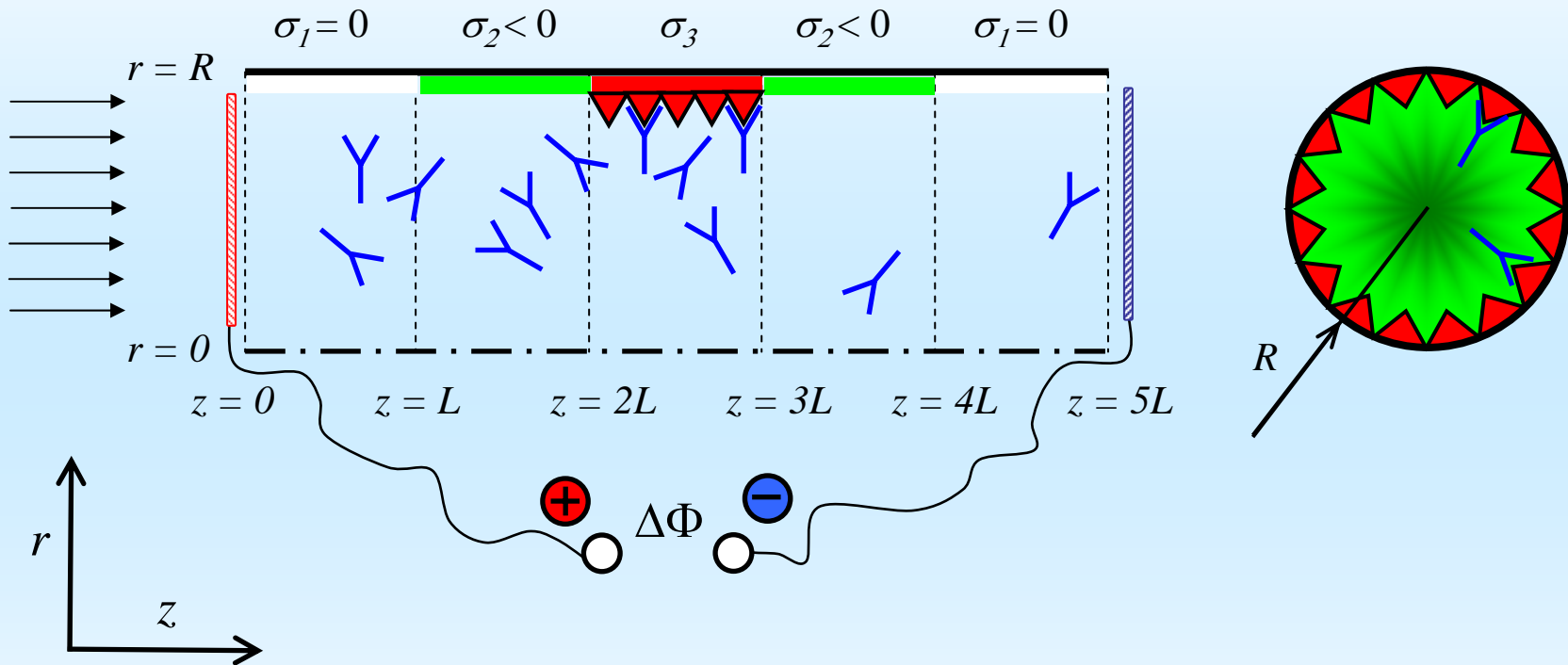
$$\vec{v}|_{wall} = 0$$

- Local deviation from electroneutrality

$$\sum_i z_i c_i \neq 0 \Rightarrow \rho_{el} \neq 0 \Rightarrow \nabla \cdot \nabla \Phi = -\frac{\rho_{el}}{\epsilon_0 \epsilon_r}$$

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# Model of a biosensor driven by an external DC electric field



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

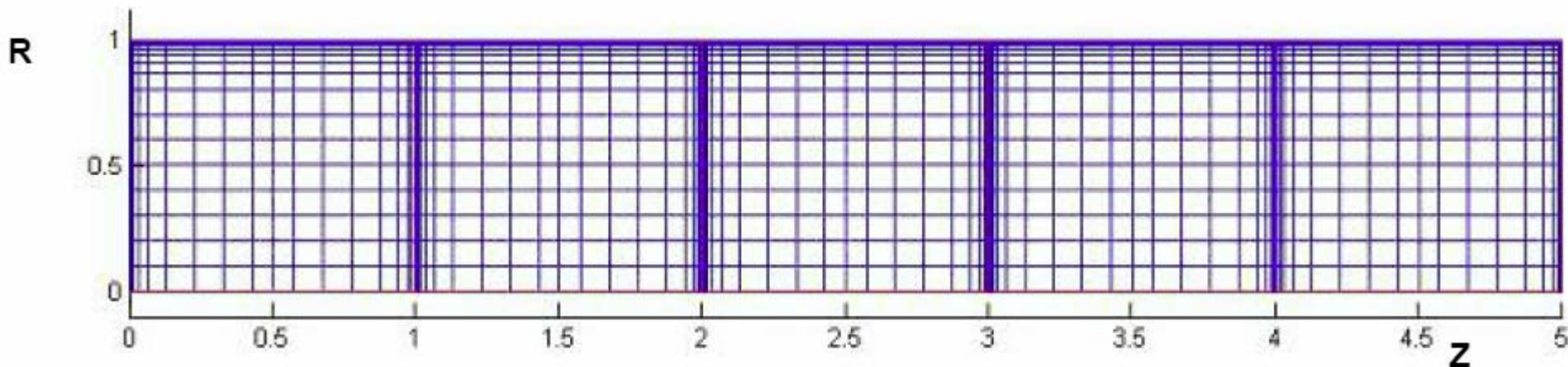
Device consists of 5 compartments  
 DC electric field is applied  
 Electric charge attached to walls



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# Meshing

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

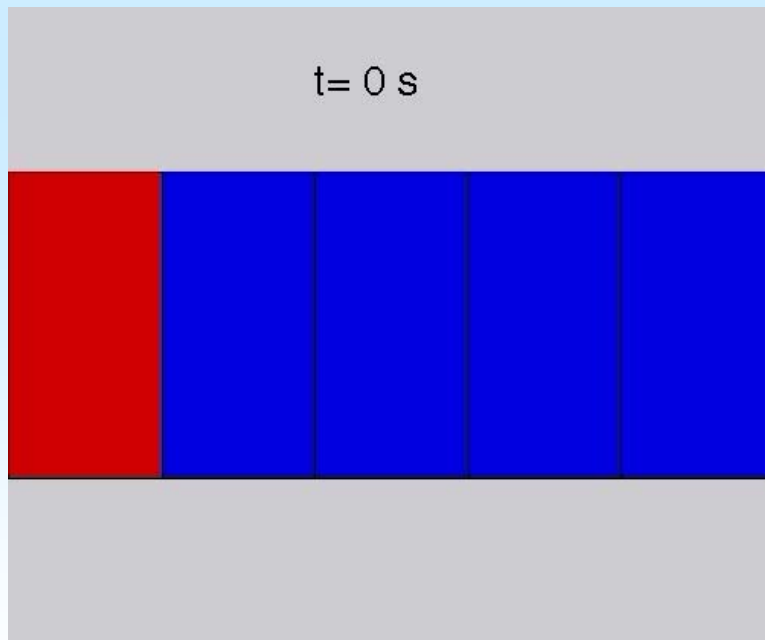


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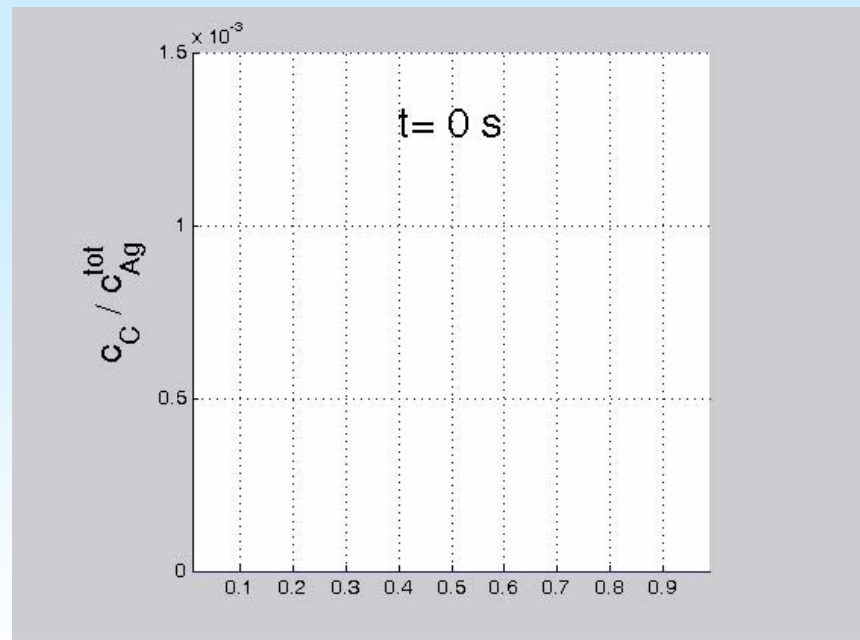
# Short-time electrokinetic dosing of a ligand in aqueous solution

Formation of the ligand-receptor complex on microchannel wall

Ligand concentration field

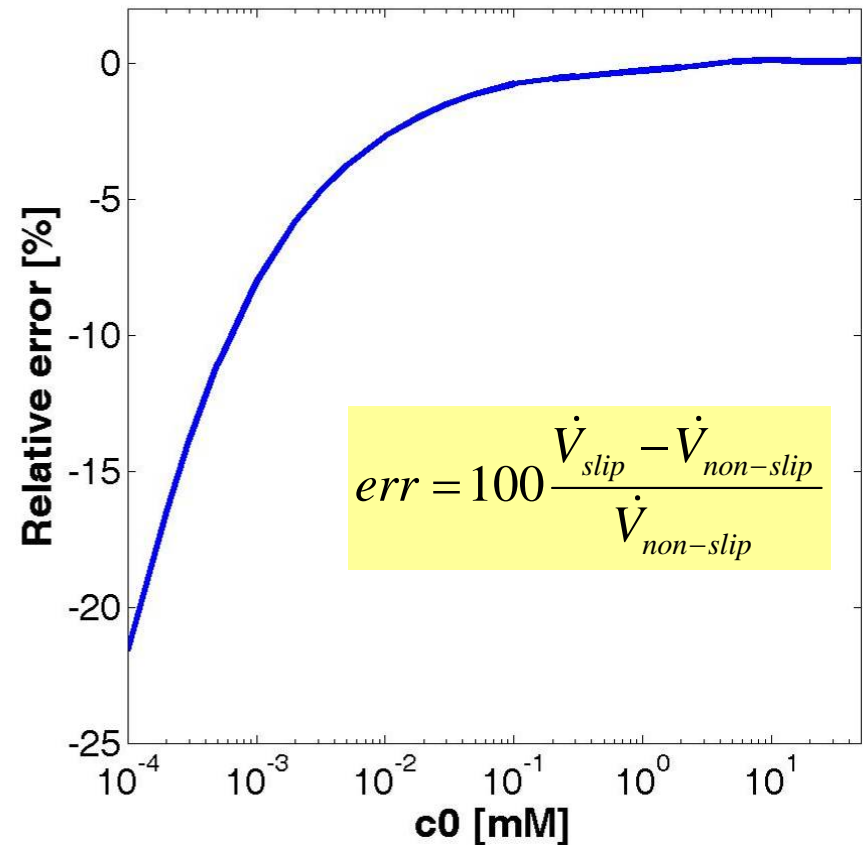
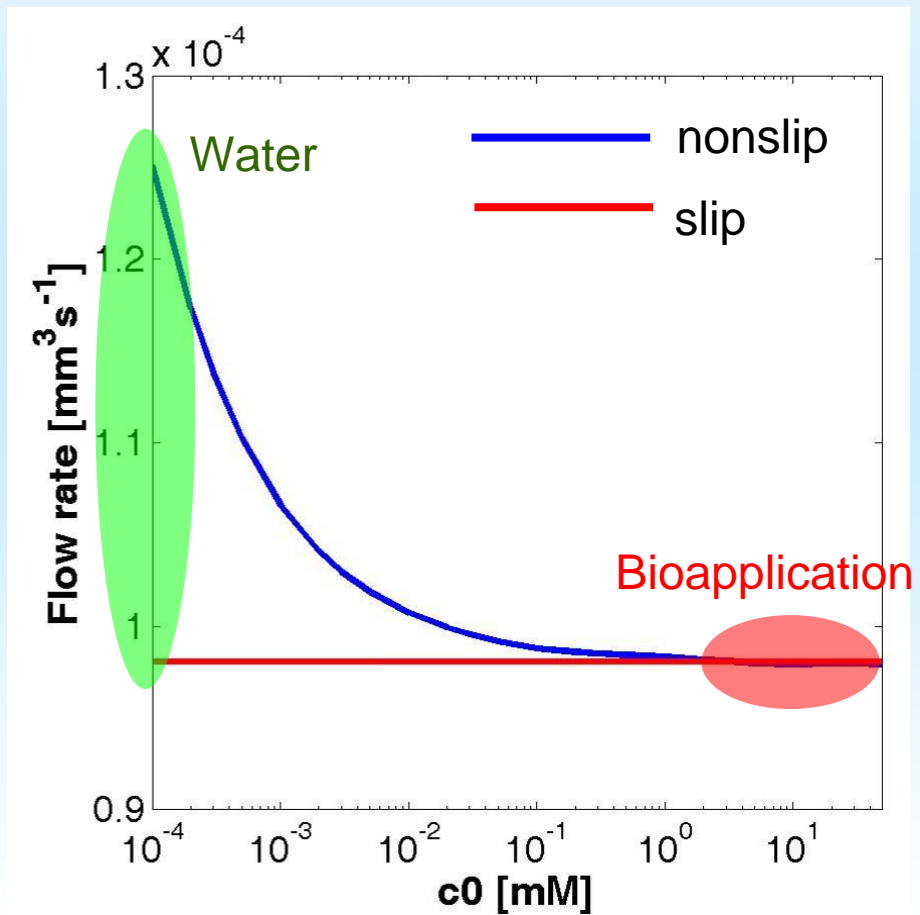


Level of saturation of the receptor binding sites



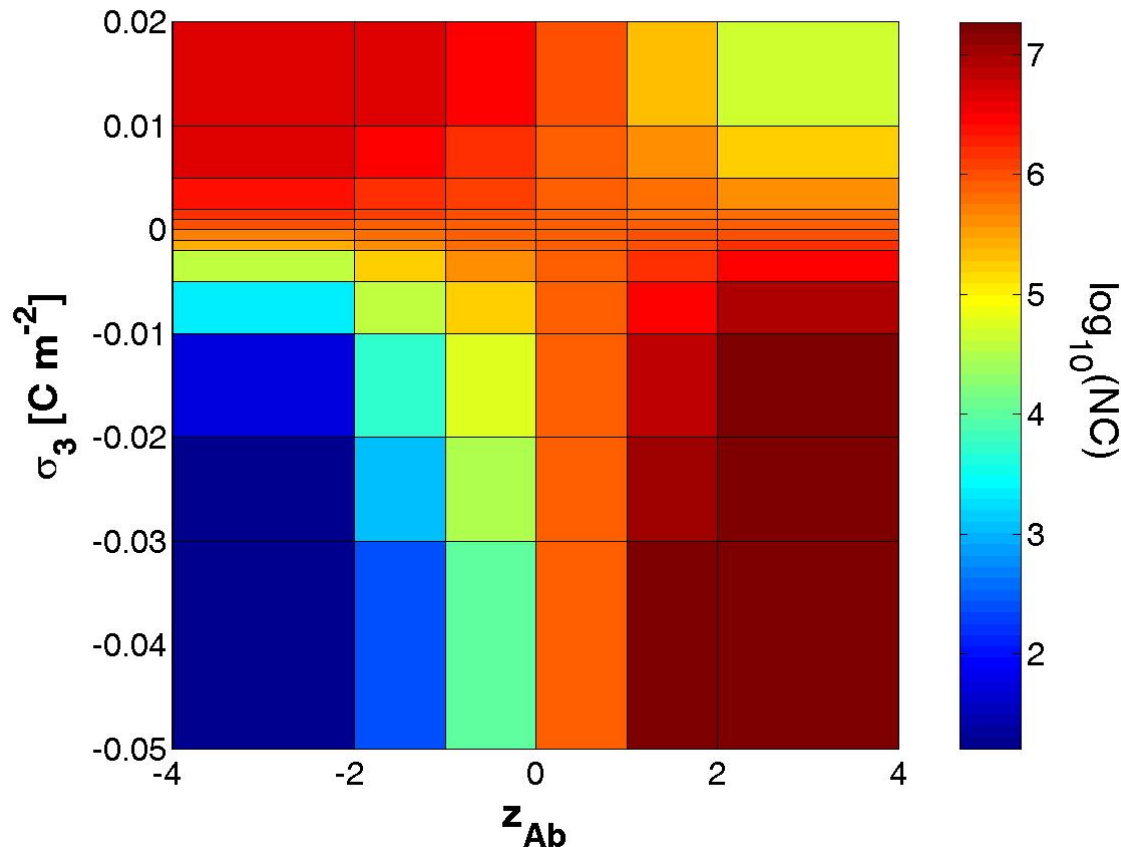
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# Example of limitation of the slip model – electrolyte concentration



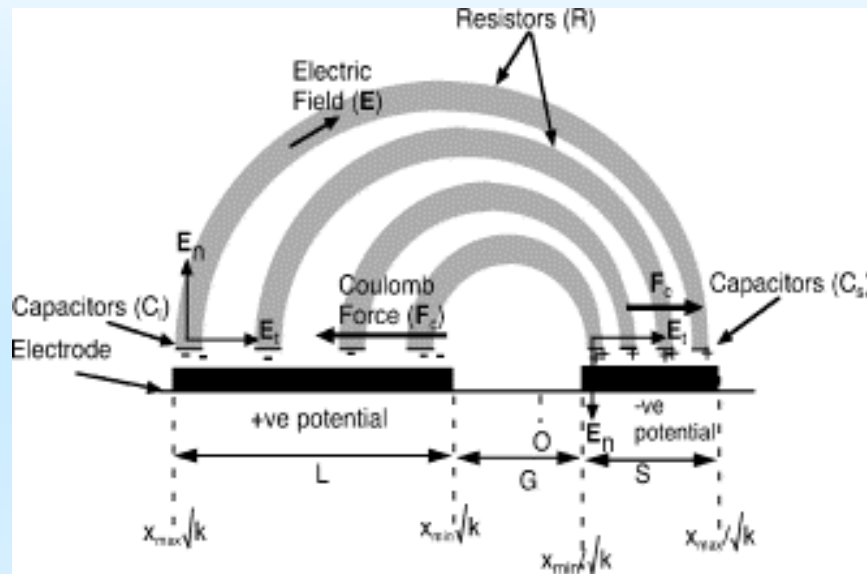
# Example of the slip model limitations – ligand-wall (receptor) electrostatic interaction

Effects of the surface electric charge  $\sigma_3$  and ligand charge number  $z_{Ab}$  on formation of ligand-receptor complex on the microchannel wall

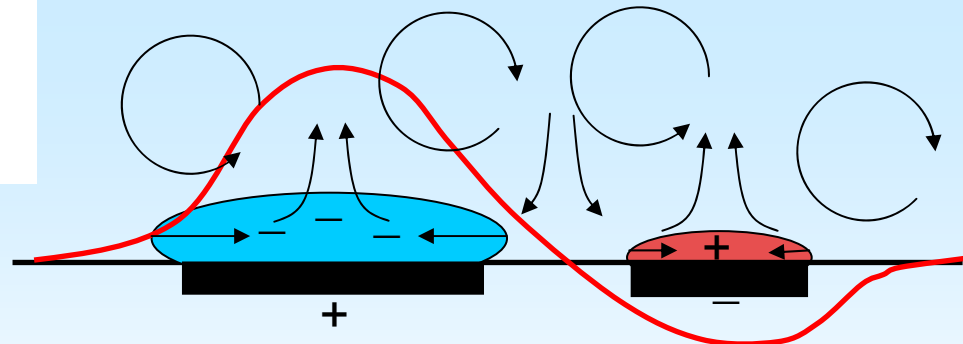


NC is the total number of molecules of the ligand-receptor complex

# Principle of AC electroosmosis



M. Mpholo, C.G. Smith, A.B.D. Brown, *Sensors and Actuators B Chemical*, 92, pp. 262-268, 2003.

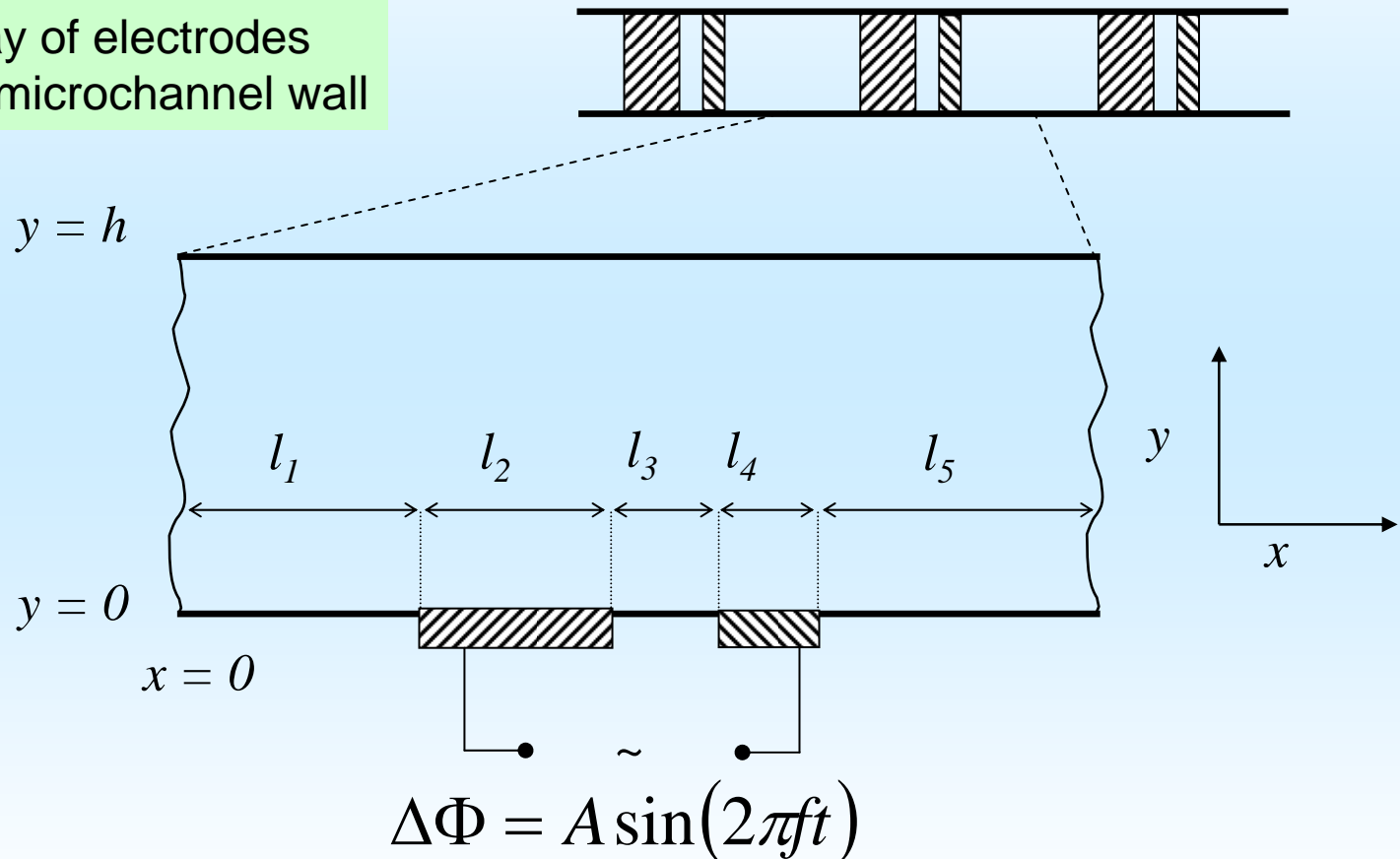


Distribution of electric potential along the electrodes (red line) induces tangential movement of the electric charge and thus eddies formation.

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

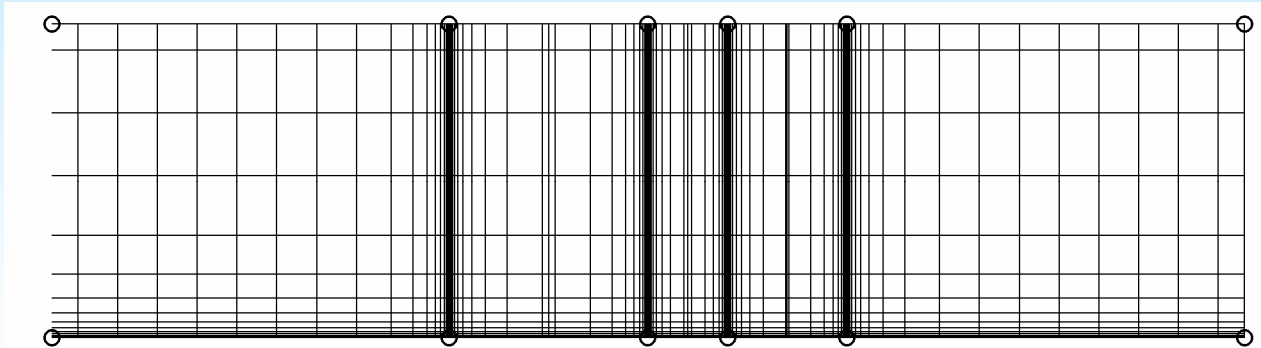
Periodic array of electrodes deposited a microchannel wall



Geometry and dimensions of the microchannel  
 ( $l_1 = l_5 = h = 10 \mu\text{m}$ ,  $l_2 = 5 \mu\text{m}$ ,  $l_3 = 2 \mu\text{m}$ ,  $l_4 = 3 \mu\text{m}$ ).

# Meshing

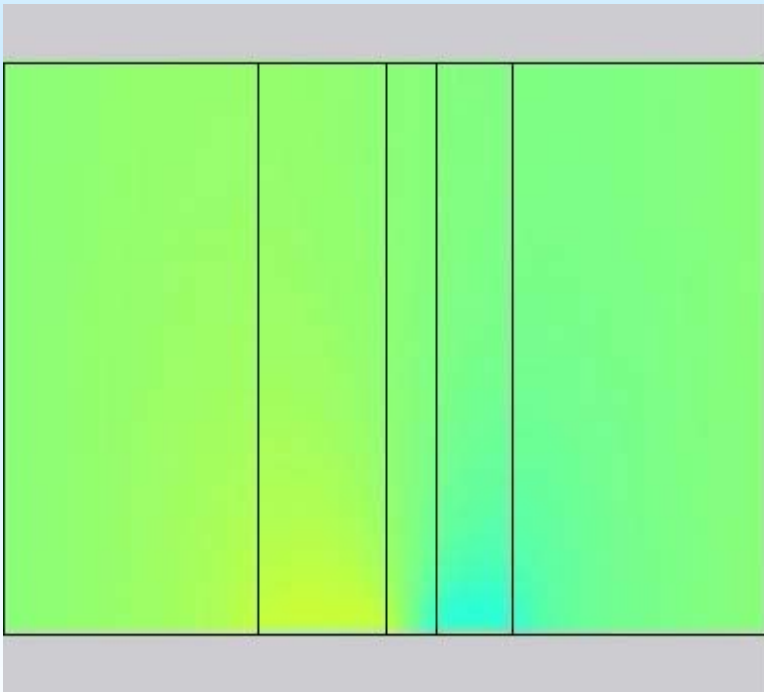
- 2800 rectangular elements
- non-equidistant
- anisotropic
- the ratio of the larger and the smaller edge of rectangles in interval  $10^0 - 2 \times 10^4$



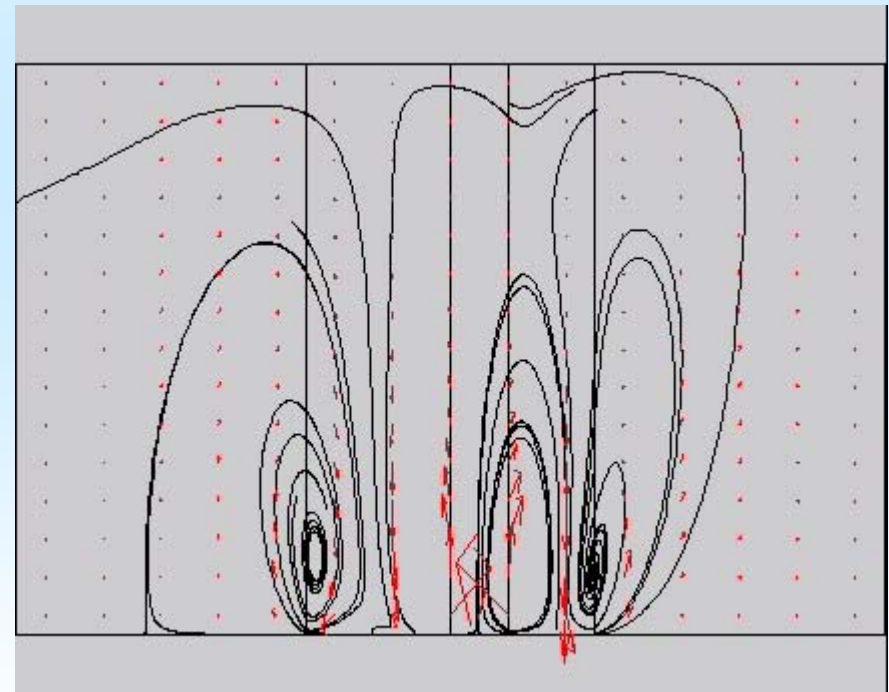
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# Steady periodic regime $A = 1$ V, $f = 1$ kHz

Electric potential distribution  
(blue  $\Delta\Phi = -1$  V, red  $\Delta\Phi = +1$  V)



Velocity distribution





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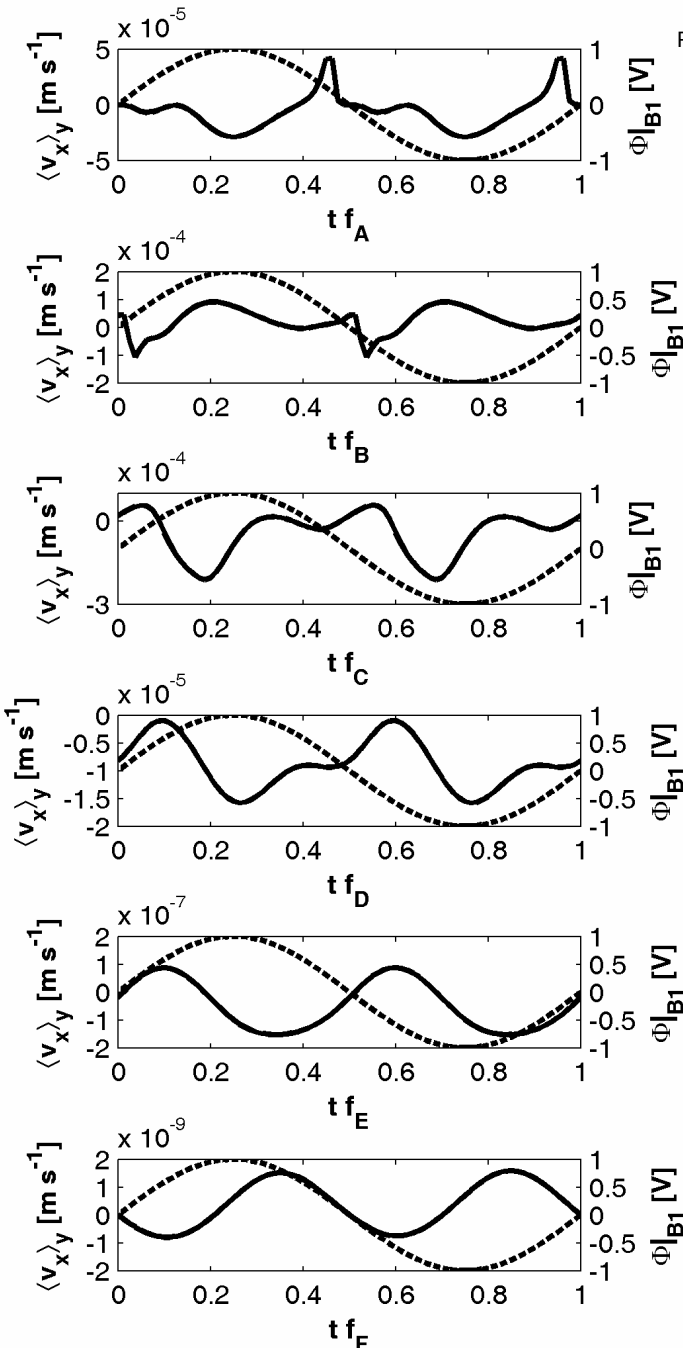
# Time course of global velocity

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  $f = 1 \times 10^4 \text{ s}^{-1}$ ) exhibits changes in flow direction during one period ( $1/f$ )  $\Rightarrow$  fluid motion in the microchannel has a zigzag character.

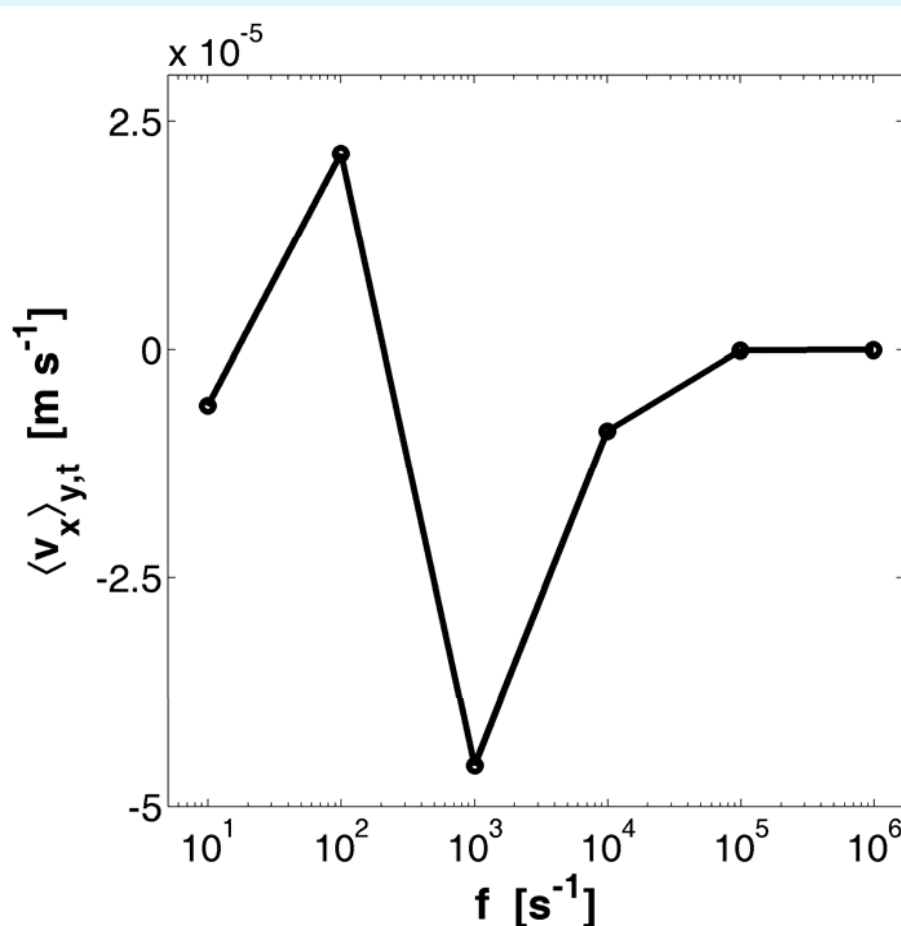
However, a continuous flux of electrolyte can be experimentally observed because of high frequency of the zigzag motion ( $2f$  or  $4f$ ).

$$f_A = 1 \times 10^1 \text{ s}^{-1}, f_B = 1 \times 10^2 \text{ s}^{-1}, f_C = 1 \times 10^3 \text{ s}^{-1}, \\ f_D = 1 \times 10^4 \text{ s}^{-1}, f_E = 1 \times 10^5 \text{ s}^{-1}, f_F = 1 \times 10^6 \text{ s}^{-1}.$$



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# Dependence of global velocity on AC frequency, $A = 1 \text{ V}$



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 second in the frequency interval  $\langle 10^2, 10^4 \rangle$  Hz.

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# 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