Technical Report

The enclosed script deals with a mathematical model of an AC electroosmotic micropump with an array of coplanar metallic microelectrodes in a zigzag arrangement. The data produced by the model are used for the analysis of AC electroosmotic flow in a micro- and nanoscale and for the optimization of the constructional and operational parameters of a future prototype. The model allows the study of dependence of the generated pumping effect on the device scale, microchannel dimensions and proportions, the driving AC field frequency and amplitude, and the applied back-pressure. Furthermore, the dynamics of the electric double layer charging can be analyzed. All variables are dimensionless, which facilitates the investigation of effects arising during the device miniaturization. The script is written for the combination of COMSOL Multiphysics (V3.3-V3.5) and Matlab (R2007-R2011). Matlab provides the simulation management and additional general purpose functions, whereas COMSOL provides the solvers and postprocessing routines.

Mathematical model

The mathematical model in dimensionless form consists of the Poisson-Nernst-Planck equations

$$0 = -\nabla \cdot (\nabla\varphi) - \frac{q}{\lambda_D^2},$$

$$\frac{1}{\lambda_D}\frac{\partial c}{\partial t} = -\nabla \cdot \mathbf{J}, \qquad \mathbf{J} = -vc - \nabla c - q\nabla\varphi,$$

$$\frac{1}{\lambda_D}\frac{\partial q}{\partial t} = -\nabla \cdot \mathbf{I}, \qquad \mathbf{I} = -vq - \nabla q - c\nabla\varphi,$$

describing the electrochemical processes in the electrolyte and the Navier-Stokes and continuity equations

$$\frac{1}{\lambda_D}\frac{1}{Sc}\frac{\partial \mathbf{v}}{\partial t} = -\nabla \cdot \left(\frac{\mathbf{vv}}{Sc} - \nabla\mathbf{v}\right) - \nabla p - \frac{Ra}{\lambda_D^2} q\nabla\varphi,$$

$$0 = -\nabla \cdot \mathbf{v}$$

governing the mass and momentum conservation.

Here φ is the electrical potential, c and q are the mean electrolyte concentration and the electric charge density, $\mathbf{v} = (u, v)$ is the velocity vector. $\mathbf{J}$ is the molar ionic flux density and $\mathbf{I}$ is the electric current density. The λ_D is the Debye length, which is related to the thickness of the electric double layer. The Ra and Sc are the Rayleigh and Schmidt numbers.

Details concerning the transformation of the equations into the dimensionless form and the description of the variables can be found in [1].

Modeling domain, discretization mesh and boundary conditions

The modeling domain is two-dimensional. The domain is divided into six parts, the bulk region and the EDL regions near the electrodes (except the situation a), when $L_e < 0.25$). This subdivision provides more control over the distribution of finite elements and allows a more detailed analysis of the EDL behavior.

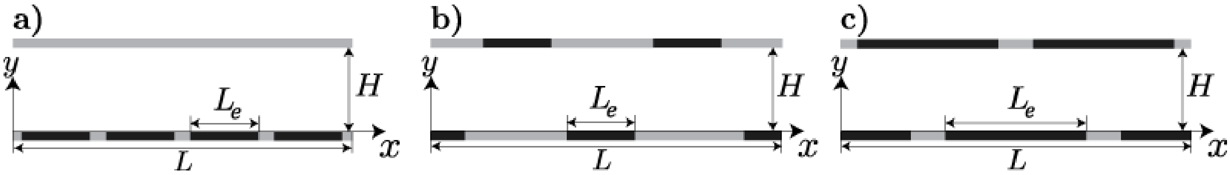

Figure 1: The modeling domain. The black and grey boxes represent the electrodes and dielectric surfaces, respectively.

The variants b) and c) refer to the situations, when the electrodes occupy bottom and top walls of the microchannel. This zigzag arrangement comprises of two interdigitated arrays of electrodes and should be easier to fabricate then the variant a). The microchannel walls between the electrodes act as hydrodynamic resistances. The zigzag arrangement allows almost full coverage of the channel walls by electrodes, which shoul result in a higher micropump performance, compared to the version a).

As mentioned before, the modeling domain is subdivided into six parts. The AC electroosmosis represent a multiscale problem, which requires a highly anisotropic discretization mesh. In the EDL subdomains, a dense structured quadrilateral mesh is used to capture the dynamics at the Debye length scale. The bulk subdomain is discretized by a sparser triangular mesh. This setup helps the convergence and reduces the demands on computer hardware resources.

The boundary conditions can be summarized as follows:

The electric potential is prescribed at the electrodes as a system of functions of time

$$\varphi_i(t) = A\sin\left(\omega t - \frac{2\pi}{4}(i-1)\right),\ i = 1,2,3,4,$$

where A is the AC voltage amplitude, $\omega = 2\pi f$ is the angular frequency, f is the AC field frequency and t is time. These functions comprise a traveling wave of the electric potential.

The electrodes and dielectric surfaces do not permit mass and charge transfer

$$\mathbf{n} \cdot \mathbf{J} = \mathbf{n} \cdot \mathbf{I} = 0$$

and the velocity vector field also vanishes at the michochannel walls

$$\mathbf{v} = (0,0).$$

The value of the pressure is fixed in left bottom corner of the modeling domain.

Sample results

The typical output given by the model is in the form of profiles. Profiles mean the distribution of model quantity in time and space. The profiles provide information about the system behavior.

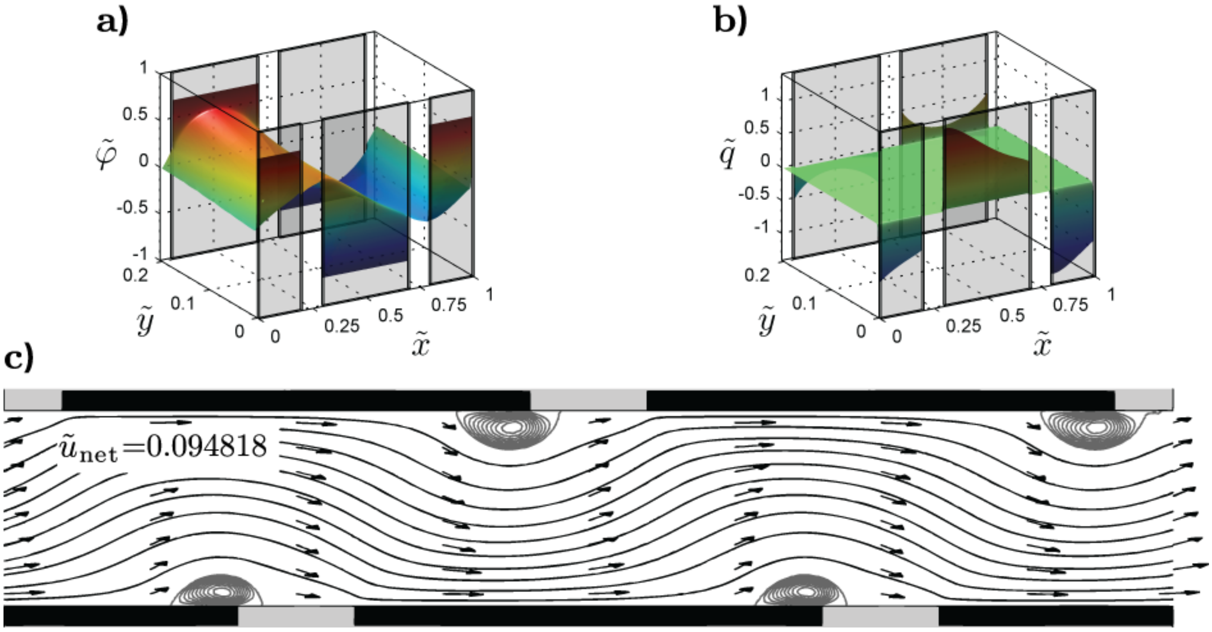

Figure 2: Profiles of system quantities at the optimal frequency and zero back-pressure: a) The electric potential; b) the electric charge density; the flow velocity. AC amplitude: 25.7 mV, L = 100 Debye lengths.

The profiles can be further postprocessed to give a more general information about the system and trends determining the system behavior under diferent conditions, such as applied back-pressure gradients (Fig. 3), increased AC voltage amplitude, changed geometry of a microfluidic channel or electrodes (Fig. 4), etc.

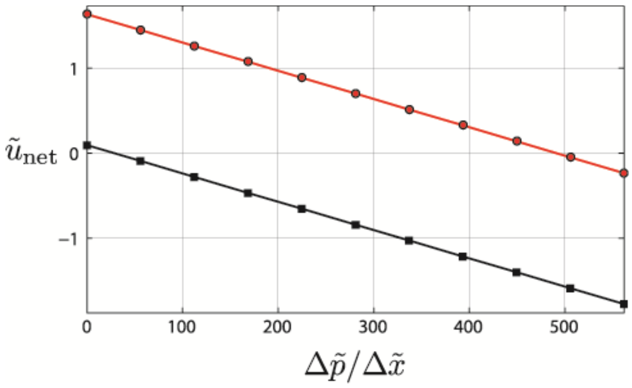

Figure 3: The dependence of the flow rate on the applied back-pressure gradient at the amplitude $A = 1$ (black line) and $A = 10$ (red line).

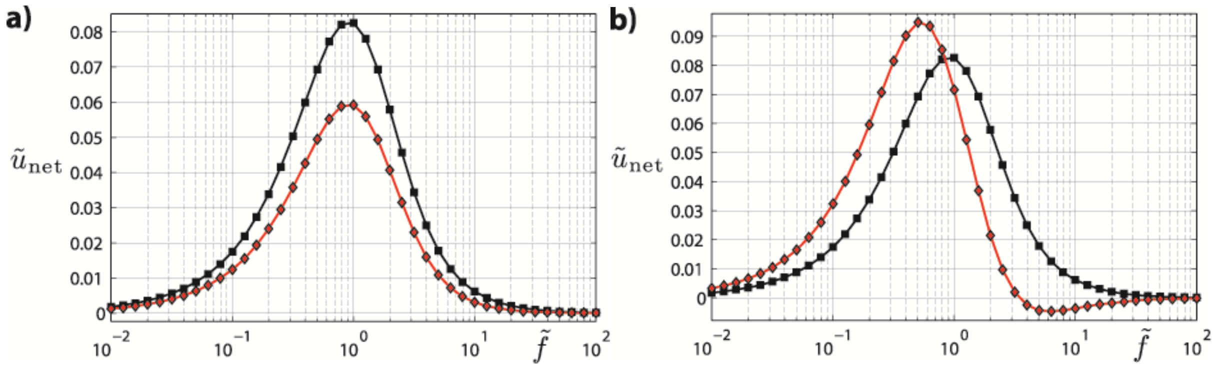

Figure 4: The dependence of the flow rate on the AC field frequency. The left plot shows the comparison of the variant 1a) (black line) and 1b) (red line) with the same length of electrodes. The right plot show the comparison of variant 1a) (black line) at L_e= 0.2 and variant 1c) at L_e = 0.4.