Technická zpráva – Software

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Název: **Software for analysis of transport processes in nanofluidic electrified systems**

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The enclosed script deals with a mathematical model of an AC electroosmotic micropump with an array of coplanar metallic microelectrodes in three- and four-phase arrangements. The data produced by the model are used for the analysis of the performance of the AC electroosmotic flow in a micro- and nanoscale. The model allows the study of the dependence of the generated pumping on a variety of model parameters, such as the microchannel dimensions and proportions, the driving AC field frequency and amplitude, and the applied back-pressure. After solution, the concentrations of the ionic species, the electric potential in the electrolyte, the velocity and pressure fields are readily available. All variables are dimensionless to facilitate the investigation of effects arising during the device miniaturization. The script is written for the combination of COMSOL Multiphysics (V3.5) and Matlab (R2008a-R2011a). Matlab provides the simulation management and additional general purpose functions, whereas COMSOL provides the solvers and postprocessing routines. All equations are transformed into the weak form to make use of all the COMSOL capabilities.

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. The third equation doubles as the continuity equation for the total electric current density $\mathbf{I}_{\mathrm{tot}}$.

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 a two-dimensional rectangle shown in Fig. 1. The domain is divided into several parts, the bulk region and the EDL regions near the electrodes. This subdivision provides more control over the distribution of finite elements and allows a more detailed analysis of the EDL behavior.

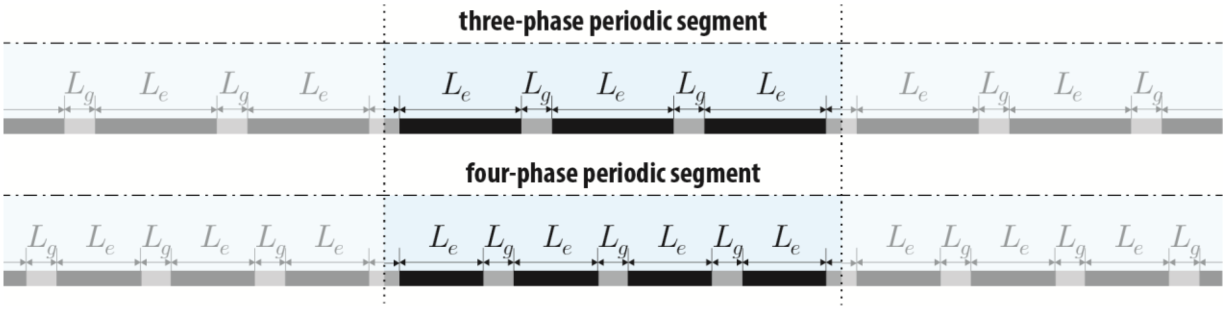

Figure 1: The modeling domain. The black and grey boxes represent the electrodes and dielectric surfaces, respectively.

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 right 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.

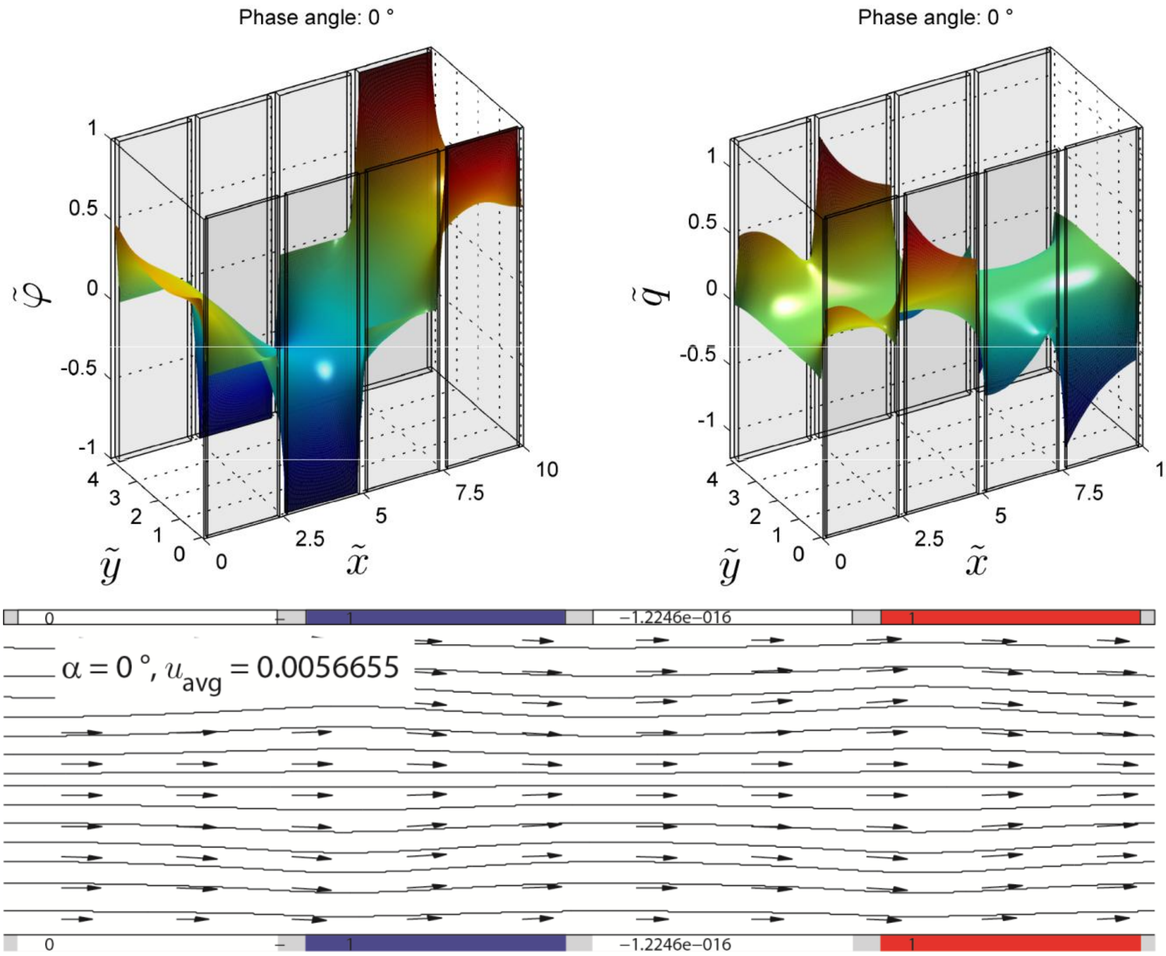

Figure 2: Profiles of system quantities at the optimal frequency and optimal back-pressure: The electric potential (top left); the electric charge density (top right); the flow velocity (bottom). AC amplitude: 25.7 mV, $\tilde{L} = 10$ Debye lengths.

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 amplitude (Fig. 3), or the arrangement of electrodes (Fig. 4), etc.

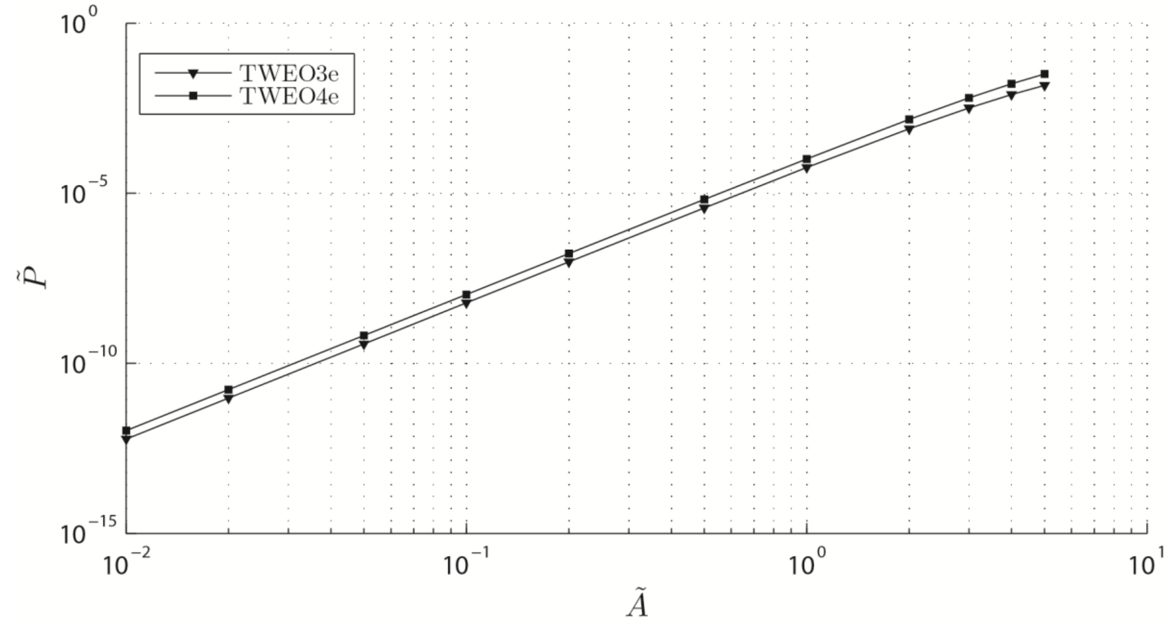

Figure 3: The dependence of the micropump performance density on the applied AC voltage amplitude $\tilde{L} = 10$ and $\tilde{H} = 4$ and the optimum back-pressure and frequency.

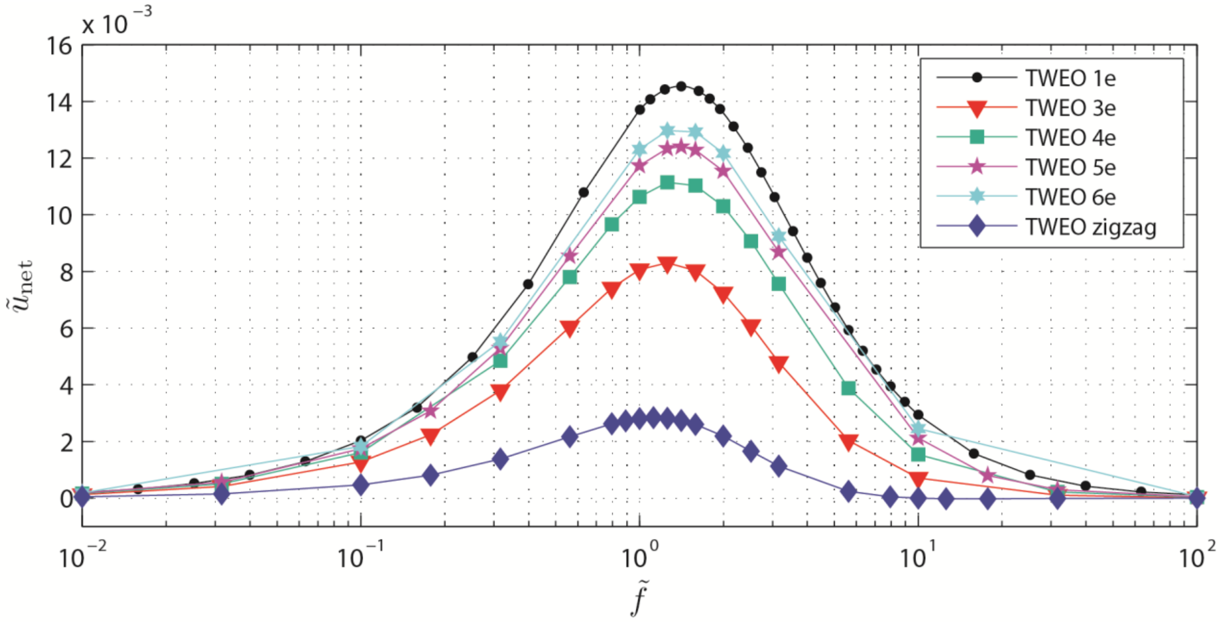

Figure 4: The dependence of the flow rate on the AC field frequency. The left plot shows the comparison of several electrode arrangements with the same length of electrodes at$\tilde{A} = 1$, $\tilde{L} = 10$, $\tilde{H} = 4$ and zero back-pressure. TWEO Ne denotes a Traveling Wave Electro-Osmotic pump with N AC phases.