NUMERICAL STUDIES OF NONLINEAR KINETICS IN INDUCED-CHARGE ELECTRO-OSMOSIS

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Summary We present a numerical study of induced-charge electro-osmosis (ICEO) of electrolytes in microfluidic channels containing a fixed dielectric structure. ICEO is the nonlinear electro-osmotic slip that occurs in the electrolyte when an applied electric field acts on the ionic charge it induces around the polarizable surface of the dielectric structure. We also establish a method for optimizing the shape of the dielectric structure for any given objective function, e.g. the resulting pumping velocity achieved for asymmetric structures.

INTRODUCTION

Induced-charge electro-osmosis (ICEO) is the nonlinear electro-osmotic slip that occurs in an electrolyte when an applied electric field acts on the ionic charge it induces around an polarizable surface of any dielectric in contact with the electrolyte. Within the past few years in microfluidics, a number of cases of nonlinear ICEO flows with both AC and DC forcing have been observed around isolated and inert (but polarizable) objects. Early examples of dielectric structures comprise flat dielectric stripes on a planar blocking electrode [1], protruding dielectric corners far from any electrode [2], and channel junctions sustaining nearby electrokinetically driven vortices [3]. More recent examples of experimental ICEO observations involve symmetric microfluidic ICEO flow [4], reduction of ICEO at high voltage bias in the nonlinear regime [5], and ICEO-based mixing in microflidc systems [6]. The ICEO flows have also been studied theoretically, from analysis of the basic basic concept [7], over a thorough treatment of the general equations [8], to a more recent detailed analysis of symmetry breaking [9].

These experimental and theoretical studies suggest that a rich variety of nonlinear electrokinetic phenomena at polarizable surfaces remains to be exploited in microfluidic devices. The aim of this paper is to advance the understanding of ICEO by numerical simulation of the nonlinear governing equations of the electrokinetics of an electrolyte in a confined microfluidic channel. We also establish a method for optimizing the shape of the dielectric structure for any given objective function, e.g. the resulting pumping velocity achieved for asymmetric structures.

MODEL AND GOVERNING EQUATIONS

We consider, as sketched in Fig. 1(a), an infinite parallel-plate capacitor with conducting yz-planes at $x = \pm L$ kept at potentials $\pm\phi_0$. Somewhere in between the plates is placed a dielectric structure, and the rest of the space is filled with an electrolyte having a viscosity η, a constant density ρ, and containing concentrations $c_\pm$ of ions with charges $\pm Ze$ and mobilities $\beta_\pm$. The whole system is translationally invariant along the z axis. The velocity and pressure fields of the electrolyte are denoted $\mathbf{u}$ and p, respectively, while the ionic current densities are denoted $\mathbf{J}_\pm$. The electric properties are described by the potential ϕ and the permittivity $\epsilon(\mathbf{r})$, which vary in space due to the presence of the dielectric structure. The governing equations of the system are modeled by the steady-state Navier–Stokes and continuity equation for incompressible fluids, the Maxwell equation for the static potential, and the Nernst–Planck and continuity equation for the ions:

$$\rho\big(\mathbf{u}\cdot\boldsymbol{\nabla}\big)\mathbf{u} = -\boldsymbol{\nabla}p + \eta\nabla^2\mathbf{u} - Ze\big(c_+ - c_-\big)\boldsymbol{\nabla}\phi, \tag{1a}$$

$$\boldsymbol{\nabla}\cdot\mathbf{u} = 0, \tag{1b}$$

$$\boldsymbol{\nabla}\cdot\big[\epsilon\boldsymbol{\nabla}\phi\big] = -Ze\big(c_+ - c_-\big), \tag{1c}$$

$$\mathbf{J}_\pm = -\beta_\pm\left(\pm c_\pm\boldsymbol{\nabla}\phi + \frac{k_\mathrm{B}T}{Ze}\boldsymbol{\nabla}c_\pm\right) + \mathbf{u}\,c_\pm, \tag{1d}$$

$$\boldsymbol{\nabla}\cdot\mathbf{J}_\pm = 0. \tag{1e}$$

RESULTS

The governing nonlinear, coupled partial differential equations have been implemented in the commercial software Comsol Multiphysics. A typical result for the resulting potential and ICEO flow field is shown in Fig. 1(b) and (d), respectively. The flow field shows a characteristic four-vortex structure also found in the analytical work by Bazant *et al.* [9]. However, as seen in Fig. 1(c) the agreement with the analytical result is only qualitative. The reason for the quantitative discrepancy is that here the fully nonlinear equations have been solved, and the system is in a confined space, while the analytical result was obtained for an unbounded electrolyte in the limit of infinitely thin Debye layers and in the linear, high-temperature Debye–Hückel limit. The advantage of our numerical method is that without the limiting approximations of the analytical

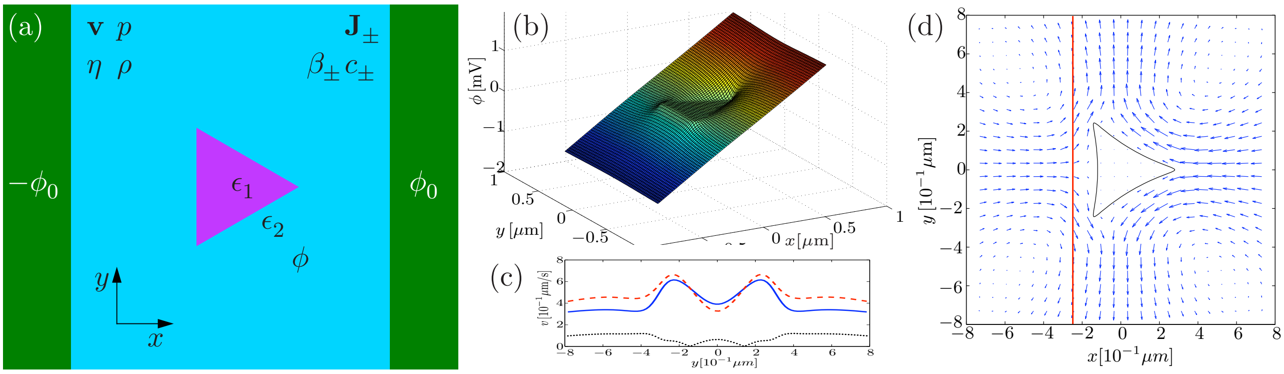

Figure 1. (a) A sketch of the model in the xy plane with the two parallel plate electrodes to the left and right, and the dielectric structure in the middle. All fields are mentioned. (b) A numerical simulation of the electric potential ϕ for a triangular dielectric structure; its shape is given by the conformal mapping $e^{i\theta} + 0.4\, e^{-i2\theta}$ of the unit circle. (c) A comparison of the numerically (red dashed line) and analytically (blue line) calculated ICEO flow velocity $|\mathbf{v}|$ along the line with parallel to the y axis through $x = -2.4$ μm. (d) A numerical simulation of the ICEO flow field in the xy plane. The red line indicates the position of the line scan in panel (c).

approach, it can form the basis for a wider range of studies, such as optimization of the system design with respect to various quantities related to ICEO. In particular we aim at maximizing the nonzero flowrate through the microfluidic channel that arises when the dielectric structure has spatial asymmetries.

To optimize the flowrate of the ICEO device we employ the method of topology optimization. This method has recently been adapted to microfluidcs and implemented in Comsol Multiphysics [10, 11]. The method relies on the introduction of an artificial porous medium in the fluidic system. The porosity is characterized by a parameter field $\gamma(\mathbf{r})$ which takes values between zero, corresponding to small pores and high friction (a wall-like structure, here the dielectric structure), to unity, corresponding to large pores and low friction (pure liquid, here the electrolyte). The parameter field couples to the governing equations through a Darcy friction force $-\alpha(\gamma(\mathbf{r}))\mathbf{v}$ added to the Navier–Stokes equation, and through the electric permittivity $\epsilon(\gamma(\mathbf{r}))$ and the mobilities $\beta_\pm(\gamma(\mathbf{r}))$. We have implemented γ-dependence of all three coefficients such that we have zero Darcy friction as well as high permittivity and conductivity for γ being unity (the liquid phase), and large Darcy friction as well as low permittivity and conductivity for γ being zero (the dielectric phase).

From an initially given $\gamma_0(\mathbf{r})$, the governing equations are solved. The objective function, here the flow rate, is calculated together with the so-called sensitivity of the system. From the latter an improved update of the parameter field $\gamma(\mathbf{r})$ is determined, and a new iteration is run. At some point the iteration converges, and in this state the parameter field is either zero or unity in most of space; hardly no intermediate values are found. As a result regions with pure liquid and with the dielectric can be identified, and thus the optimal shape of the dielectric structure can be determined.

CONCLUSIONS

We have established a numerical method by using Comsol Multiphysics that allows us to calculate the ICEO flow resulting from nonlinear kinetics in complex geometries, i.e. for arbitrarily shaped dielectric structures in microfluidic channels with electrolytes. We have introduced a continuous parameter field $\gamma(\mathbf{r})$, by which regions of pure electrolyte and of dielectric material can be identified and changed. One such calculation forms a single step in the iterative method of topology optimization. Using that it will be possible to explore the rich physics in the complex nonlinear ICEO flows and in particular to find optimized geometrical shapes of the dielectric to obtain maximal ICEO pumping.

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